

**Mono- and binuclear chloride complexes of bismuth(III)  
with 2-aminopyrimidine cations depending on specific synthetic route**

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**<sup>1</sup>H NMR data** (200 MHz, DMSO-d<sub>6</sub>) for the samples of compounds **1** and **2** prepared according to the different procedures.

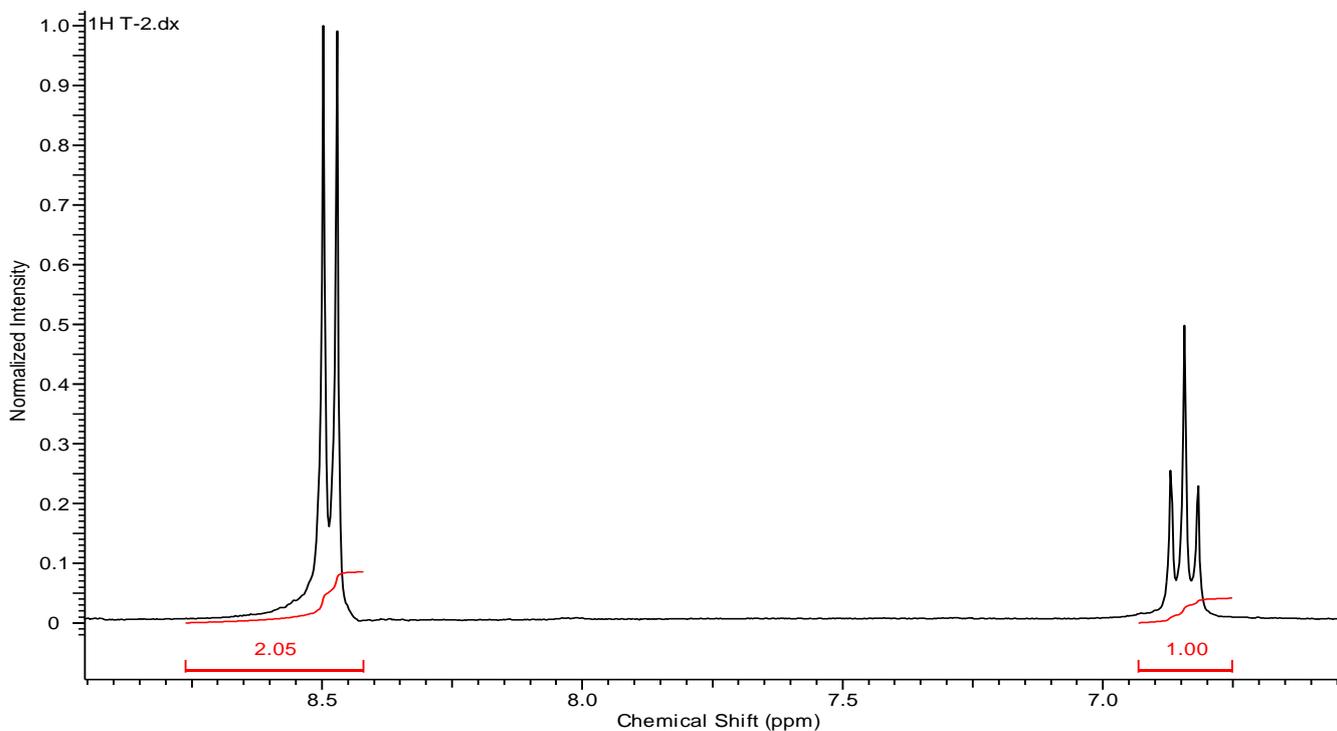
Compound **2**, synthesis in aqueous HCl, Bi : 2-AP reagent ratio of 1 : 2,  $\delta$ : 6.98 (<sup>1</sup>H, t,  $J$  = 4.7 Hz, H<sub>arom</sub>), 8.67 (2H, d,  $J$  = 4.7 Hz, H<sub>arom</sub>).

Compound **1**, conversion of compound **2** into **1**,  $\delta$ : 6.84 (<sup>1</sup>H, t,  $J$  = 4.8 Hz, H<sub>arom</sub>), 8.48 (2H, d,  $J$  = 4.8 Hz, H<sub>arom</sub>).

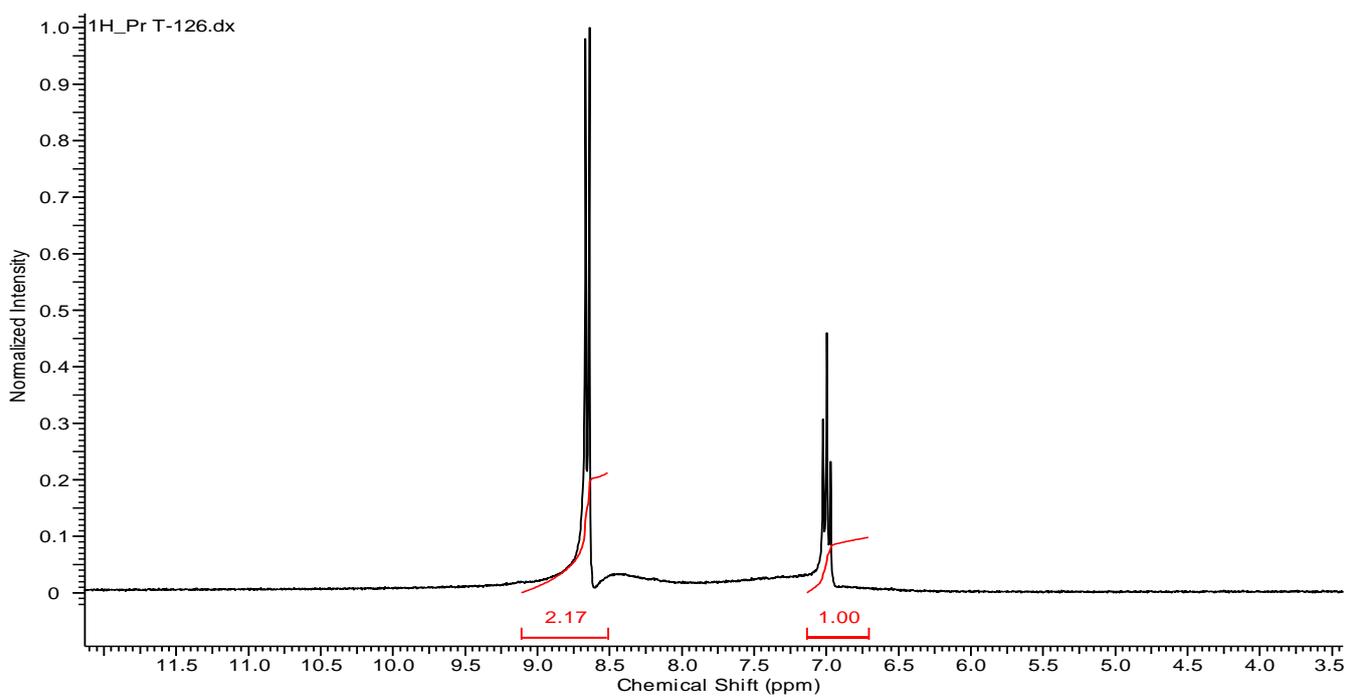
Compound **2**, synthesis in aqueous HCl, Bi : 2-AP reagent ratio of 1 : 3,  $\delta$ : 6.92 (<sup>1</sup>H, t,  $J$  = 4.7 Hz, H<sub>arom</sub>), 8.57 (2H, d,  $J$  = 4.7 Hz, H<sub>arom</sub>).

Compound **1**, synthesis in EtOH, Bi : 2-AP reagent ratio of 1 : 3,  $\delta$ : 6.97 (<sup>1</sup>H, t,  $J$  = 4.8 Hz, H<sub>arom</sub>), 8.68 (2H, d,  $J$  = 4.8 Hz, H<sub>arom</sub>).

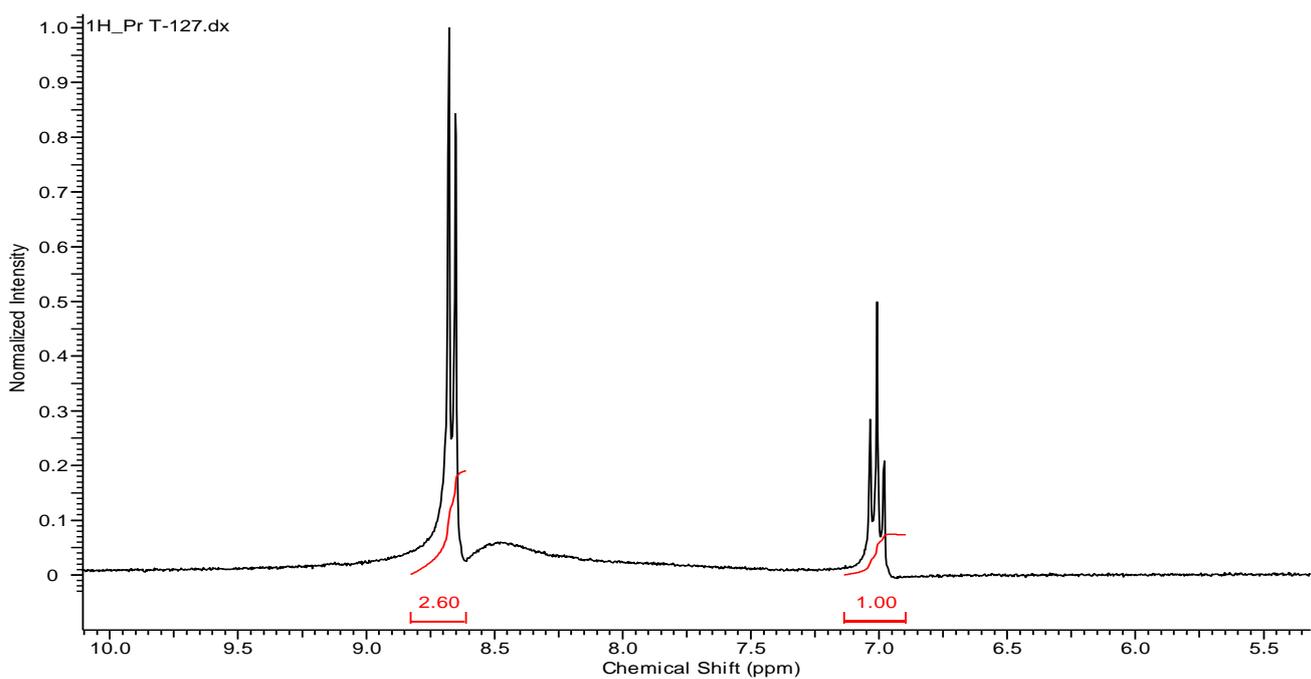
Compound **1**, synthesis in EtOH, Bi : 2-AP reagent ratio of 1 : 2,  $\delta$ : 6.96 (<sup>1</sup>H, t,  $J$  = 4.8 Hz, H<sub>arom</sub>), 8.62 (2H, d,  $J$  = 4.8 Hz, H<sub>arom</sub>).



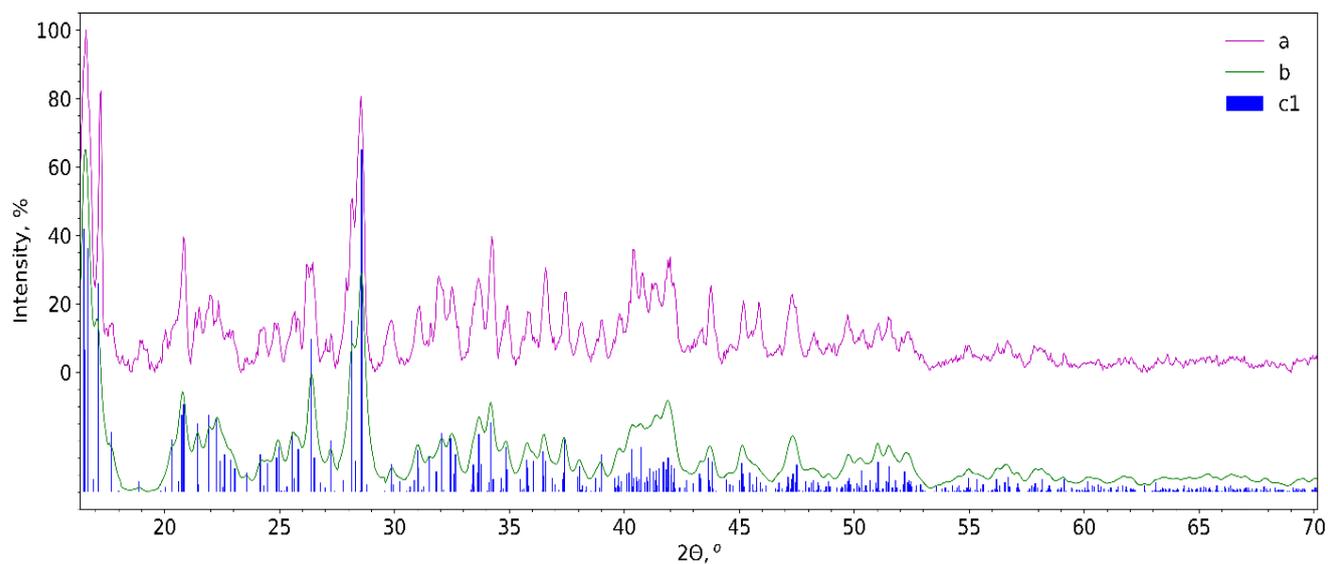
**Figure S1** <sup>1</sup>H NMR of compound **1** (Bi : 2-AP = 1 : 3).



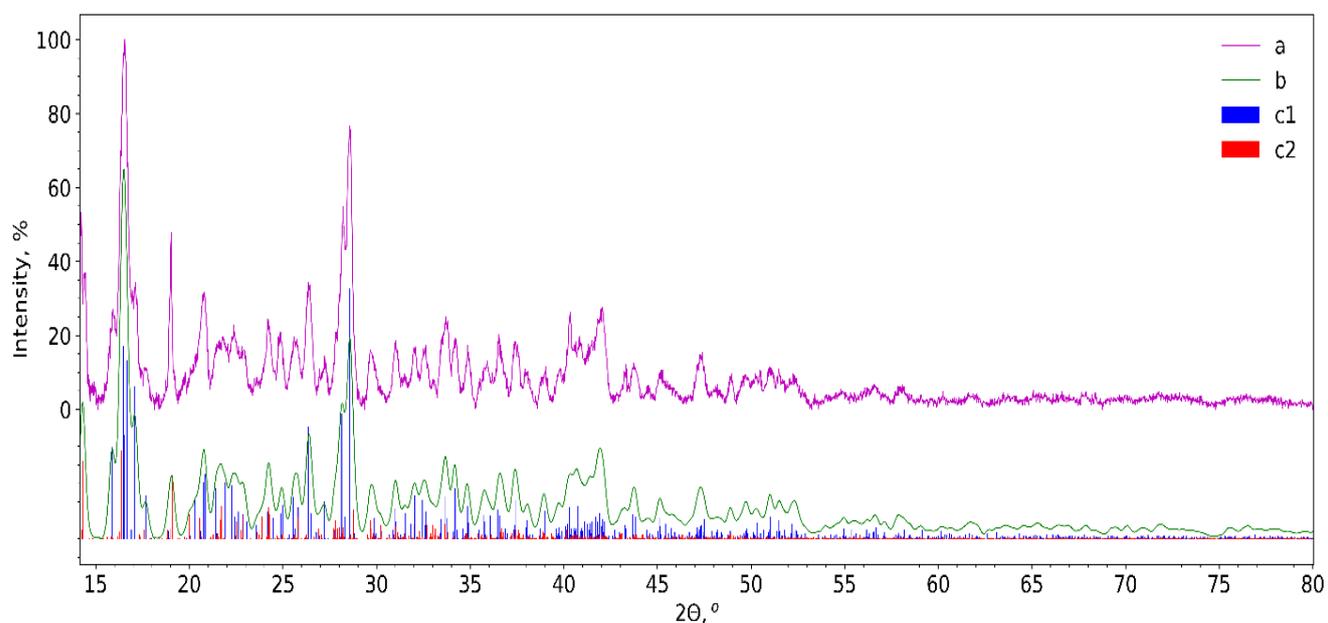
**Figure S2** <sup>1</sup>H NMR of compound 2 (Bi : 2-AP = 1 : 2).



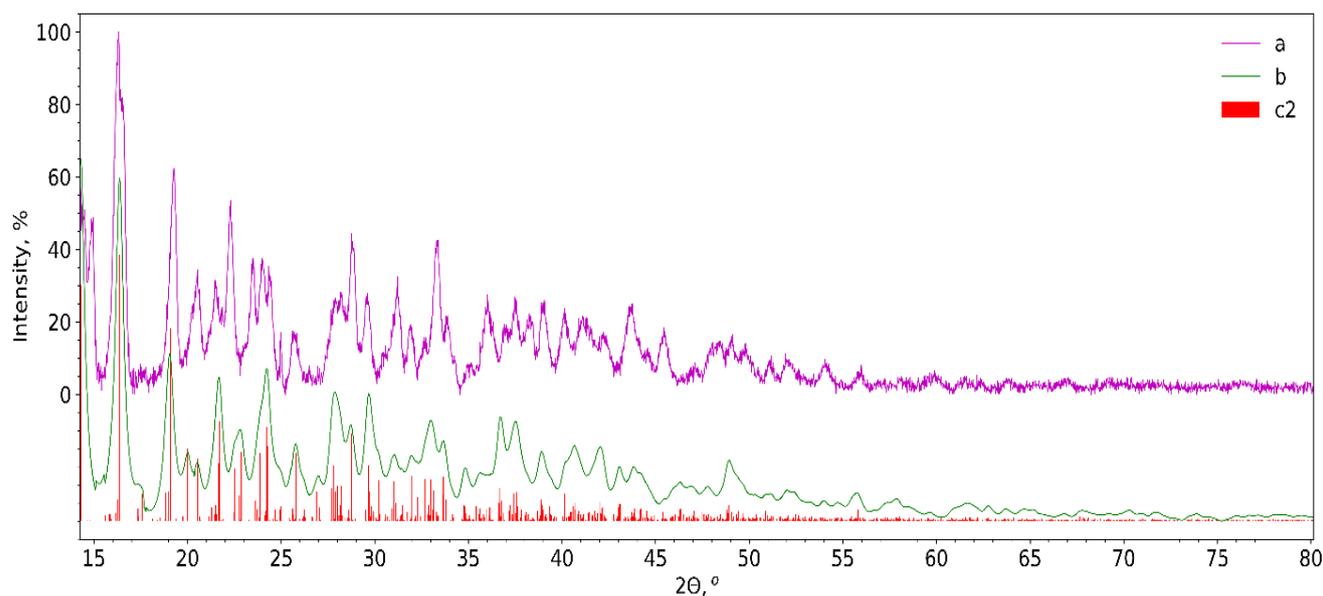
**Figure S3** <sup>1</sup>H NMR of compound 2 (Bi : 2-AP = 1 : 2).



**Figure S4 (a)** An experimental XRD pattern for sample obtained in aqueous HCl at the Bi : 2-AP regent ratio of 1 : 2 and **(b)** a theoretical diffraction pattern describing it for (c1) compound **2**.



**Figure S5 (a)** An experimental XRD pattern for sample obtained in aqueous HCl at the Bi : 2-AP regent ratio of 1 : 3 and **(b)** a theoretical diffraction pattern describing it including compounds (c1) **2** and (c2) **1** at their ratio of 67.7 : 32.3.



**Figure S6** (a) An experimental XRD pattern for sample obtained during conversion of compound **2** into **1** and (b) a theoretical diffraction pattern describing it for (c2) compound **1**.

*X-ray powder diffraction* of the produced samples was carried out using an automatic X-ray diffractometer DR-01 RADIANT ( $\text{Cu}_{K\alpha}$  radiation,  $\lambda=1.54051 \text{ \AA}$ ). The measurements were performed at room temperature in the angular range of  $14^\circ < 2\theta < 80^\circ$  with  $0.022^\circ$  resolution. The obtained XDR patterns were refined using STOE WinXPOW and original software. For this purpose, data on the structure of compounds obtained by the method of X-ray structural analysis as indicated above were used.

### X-ray crystallographic data

**Table S1** Crystal data and structure refinement for **1**.

Identification code	t752	
Empirical formula	$\text{C}_{12} \text{H}_{18} \text{Bi Cl}_6 \text{N}_9$	
Formula weight	710.03	
Temperature	295(2) K	
Wavelength	0.71073 $\text{\AA}$	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	$a = 24.7839(5) \text{ \AA}$	$\alpha = 90^\circ$ .
	$b = 7.52840(10) \text{ \AA}$	$\beta = 91.456(2)^\circ$ .
	$c = 24.7393(5) \text{ \AA}$	$\gamma = 90^\circ$ .
Volume	$4614.45(15) \text{ \AA}^3$	

Z	8
Density (calculated)	2.044 Mg/m <sup>3</sup>
Absorption coefficient	8.355 mm <sup>-1</sup>
F(000)	2704
Crystal size	.33 x .16 x .15 mm <sup>3</sup>
Theta range for data collection	1.644 to 27.811°.
Index ranges	-32<=h<=32, -9<=k<=9, -32<=l<=32
Reflections collected	113159
Independent reflections	21179 [R(int) = 0.1042]
Completeness to theta = 25.242°	100.0 %
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	21179 / 1 / 998
Goodness-of-fit on F <sup>2</sup>	0.821
Final R indices [I>2sigma(I)]	R1 = 0.0512, wR2 = 0.0972
R indices (all data)	R1 = 0.1321, wR2 = 0.1532
Absolute structure parameter	-0.015(10)
Extinction coefficient	0.00203(9)
Largest diff. peak and hole	1.401 and -1.780 e.Å <sup>-3</sup>

**Table S2** Crystal data and structure refinement for **2**.

Identification code	t751
Empirical formula	C <sub>8</sub> H <sub>12</sub> Bi Cl <sub>5</sub> N <sub>6</sub>
Formula weight	578.47
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 8.8840(3) Å      α = 114.815(3)°. b = 10.0229(4) Å      β = 108.674(3)°. c = 11.1040(4) Å      γ = 91.409(3)°.
Volume	835.54(6) Å <sup>3</sup>
Z	2
Density (calculated)	2.299 Mg/m <sup>3</sup>
Absorption coefficient	11.348 mm <sup>-1</sup>
F(000)	540
Crystal size	.22 x .20 x .15 mm <sup>3</sup>
Theta range for data collection	2.170 to 28.204°.
Index ranges	-11<=h<=11, -13<=k<=13, -14<=l<=14
Reflections collected	23529
Independent reflections	4007 [R(int) = 0.0589]

Completeness to theta = 25.242°	99.6 %
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	4007 / 0 / 182
Goodness-of-fit on F <sup>2</sup>	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0360, wR2 = 0.0778
R indices (all data)	R1 = 0.0594, wR2 = 0.1261
Extinction coefficient	0.0282(14)
Largest diff. peak and hole	1.571 and -1.912 e.Å <sup>-3</sup>

**Table S3** Torsion angles [°] for **1**.

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N(1A)-C(1A)-N(2A)-C(3A)	177(3)
N(6A)-C(1A)-N(2A)-C(3A)	0.0
C(1A)-N(2A)-C(3A)-C(4A)	0.0
N(2A)-C(3A)-C(4A)-C(5A)	0.0
C(3A)-C(4A)-C(5A)-N(6A)	0.0
C(4A)-C(5A)-N(6A)-C(1A)	0.0
N(1A)-C(1A)-N(6A)-C(5A)	-177(3)
N(2A)-C(1A)-N(6A)-C(5A)	0.0
N(6B)-C(1B)-N(2B)-C(3B)	0(6)
N(1B)-C(1B)-N(2B)-C(3B)	180(4)
C(1B)-N(2B)-C(3B)-C(4B)	1(7)
N(2B)-C(3B)-C(4B)-C(5B)	0(7)
C(3B)-C(4B)-C(5B)-N(6B)	-2(7)
C(4B)-C(5B)-N(6B)-C(1B)	2(7)
N(2B)-C(1B)-N(6B)-C(5B)	-1(7)
N(1B)-C(1B)-N(6B)-C(5B)	179(5)
N(1C)-C(1C)-N(2C)-C(3C)	176(3)
N(6C)-C(1C)-N(2C)-C(3C)	0(5)
C(1C)-N(2C)-C(3C)-C(4C)	2(6)
N(2C)-C(3C)-C(4C)-C(5C)	-3(6)
C(3C)-C(4C)-C(5C)-N(6C)	3(7)
C(4C)-C(5C)-N(6C)-C(1C)	-1(5)
N(2C)-C(1C)-N(6C)-C(5C)	0(5)
N(1C)-C(1C)-N(6C)-C(5C)	-177(3)
N(1D)-C(1D)-N(2D)-C(3D)	178(4)
N(6D)-C(1D)-N(2D)-C(3D)	-1(5)
C(1D)-N(2D)-C(3D)-C(4D)	0(6)
N(2D)-C(3D)-C(4D)-C(5D)	5(7)
C(3D)-C(4D)-C(5D)-N(6D)	-7(7)

N(1D)-C(1D)-N(6D)-C(5D)	180(4)
N(2D)-C(1D)-N(6D)-C(5D)	-1(5)
C(4D)-C(5D)-N(6D)-C(1D)	6(7)
N(6E)-C(1E)-N(2E)-C(3E)	3(6)
N(1E)-C(1E)-N(2E)-C(3E)	-176(4)
C(1E)-N(2E)-C(3E)-C(4E)	-1(6)
N(2E)-C(3E)-C(4E)-C(5E)	-1(6)
C(3E)-C(4E)-C(5E)-N(6E)	2(6)
N(1E)-C(1E)-N(6E)-C(5E)	176(4)
N(2E)-C(1E)-N(6E)-C(5E)	-3(5)
C(4E)-C(5E)-N(6E)-C(1E)	1(5)
N(1F)-C(1F)-N(2F)-C(3F)	179(3)
N(6F)-C(1F)-N(2F)-C(3F)	-2(5)
C(1F)-N(2F)-C(3F)-C(4F)	3(6)
N(2F)-C(3F)-C(4F)-C(5F)	-2(6)
C(3F)-C(4F)-C(5F)-N(6F)	1(5)
N(1F)-C(1F)-N(6F)-C(5F)	-180(3)
N(2F)-C(1F)-N(6F)-C(5F)	1(5)
C(4F)-C(5F)-N(6F)-C(1F)	-1(5)
N(1G)-C(1G)-N(2G)-C(3G)	-176(3)
N(6G)-C(1G)-N(2G)-C(3G)	3(5)
C(1G)-N(2G)-C(3G)-C(4G)	-3(6)
N(2G)-C(3G)-C(4G)-C(5G)	2(8)
C(3G)-C(4G)-C(5G)-N(6G)	-3(7)
N(1G)-C(1G)-N(6G)-C(5G)	175(4)
N(2G)-C(1G)-N(6G)-C(5G)	-5(5)
C(4G)-C(5G)-N(6G)-C(1G)	4(7)
N(1H)-C(1H)-N(2H)-C(3H)	-179(6)
N(6H)-C(1H)-N(2H)-C(3H)	3(7)
C(1H)-N(2H)-C(3H)-C(4H)	-1(7)
N(2H)-C(3H)-C(4H)-C(5H)	-1(8)
C(3H)-C(4H)-C(5H)-N(6H)	2(10)
C(4H)-C(5H)-N(6H)-C(1H)	0(9)
N(1H)-C(1H)-N(6H)-C(5H)	179(6)
N(2H)-C(1H)-N(6H)-C(5H)	-2(7)
N(1I)-C(1I)-N(2I)-C(3I)	-179(3)
N(6I)-C(1I)-N(2I)-C(3I)	0(5)
C(1I)-N(2I)-C(3I)-C(4I)	2(5)
N(2I)-C(3I)-C(4I)-C(5I)	-4(5)
C(3I)-C(4I)-C(5I)-N(6I)	4(5)

C(4I)-C(5I)-N(6I)-C(1I)	-2(5)
N(2I)-C(1I)-N(6I)-C(5I)	0(6)
N(1I)-C(1I)-N(6I)-C(5I)	179(3)
N(1J)-C(1J)-N(2J)-C(3J)	177(3)
N(6J)-C(1J)-N(2J)-C(3J)	1(5)
C(1J)-N(2J)-C(3J)-C(4J)	-3(5)
N(2J)-C(3J)-C(4J)-C(5J)	3(5)
C(3J)-C(4J)-C(5J)-N(6J)	-2(5)
C(4J)-C(5J)-N(6J)-C(1J)	1(5)
N(1J)-C(1J)-N(6J)-C(5J)	-176(3)
N(2J)-C(1J)-N(6J)-C(5J)	0(4)
N(1K)-C(1K)-N(2K)-C(3K)	-179(3)
N(6K)-C(1K)-N(2K)-C(3K)	-2(4)
C(1K)-N(2K)-C(3K)-C(4K)	3(5)
N(2K)-C(3K)-C(4K)-C(5K)	-3(5)
C(3K)-C(4K)-C(5K)-N(6K)	3(5)
C(4K)-C(5K)-N(6K)-C(1K)	-3(5)
N(2K)-C(1K)-N(6K)-C(5K)	2(5)
N(1K)-C(1K)-N(6K)-C(5K)	179(3)
N(6L)-C(1L)-N(2L)-C(3L)	1(5)
N(1L)-C(1L)-N(2L)-C(3L)	-178(3)
C(1L)-N(2L)-C(3L)-C(4L)	5(6)
N(2L)-C(3L)-C(4L)-C(5L)	-8(6)
C(3L)-C(4L)-C(5L)-N(6L)	5(6)
N(2L)-C(1L)-N(6L)-C(5L)	-4(5)
N(1L)-C(1L)-N(6L)-C(5L)	176(3)
C(4L)-C(5L)-N(6L)-C(1L)	1(5)

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**Table S4.** Torsion angles [ $^{\circ}$ ] for **2**.

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C(2A)-N(2A)-C(1A)-N(1A)	178.5(11)
C(2A)-N(2A)-C(1A)-N(3A)	-1.7(16)
C(4A)-N(3A)-C(1A)-N(1A)	-178.9(10)
C(4A)-N(3A)-C(1A)-N(2A)	1.3(15)
C(1A)-N(2A)-C(2A)-C(3A)	0.8(17)
N(2A)-C(2A)-C(3A)-C(4A)	0.4(16)
C(1A)-N(3A)-C(4A)-C(3A)	-0.1(16)
C(2A)-C(3A)-C(4A)-N(3A)	-0.7(17)
C(2B)-N(2B)-C(1B)-N(1B)	-178.0(10)
C(2B)-N(2B)-C(1B)-N(3B)	1.5(15)

C(4B)-N(3B)-C(1B)-N(1B)	177.9(11)
C(4B)-N(3B)-C(1B)-N(2B)	-1.6(16)
C(1B)-N(2B)-C(2B)-C(3B)	0.5(17)
N(2B)-C(2B)-C(3B)-C(4B)	-2.3(18)
C(1B)-N(3B)-C(4B)-C(3B)	-0.3(17)
C(2B)-C(3B)-C(4B)-N(3B)	2.1(17)

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Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+2

**Table S5.** Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **1**.

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Bi(1)-Cl(5)	2.662(9)
Bi(1)-Cl(4)	2.679(9)
Bi(1)-Cl(6)	2.693(8)
Bi(1)-Cl(2)	2.695(8)
Bi(1)-Cl(3)	2.727(10)
Bi(1)-Cl(1)	2.790(9)
Bi(2)-Cl(8)	2.568(9)
Bi(2)-Cl(10)	2.606(9)
Bi(2)-Cl(12)	2.690(8)
Bi(2)-Cl(11)	2.695(8)
Bi(2)-Cl(9)	2.869(9)
Bi(2)-Cl(7)	2.960(9)
Bi(3)-Cl(13)	2.590(9)
Bi(3)-Cl(17)	2.622(9)
Bi(3)-Cl(14)	2.668(8)
Bi(3)-Cl(16)	2.698(8)
Bi(3)-Cl(15)	2.809(9)
Bi(3)-Cl(22)	2.911(9)
Bi(4)-Cl(24)	2.627(9)
Bi(4)-Cl(18)	2.674(8)
Bi(4)-Cl(23)	2.684(9)
Bi(4)-Cl(19)	2.706(10)
Bi(4)-Cl(21)	2.715(8)
Bi(4)-Cl(20)	2.813(9)
N(1A)-C(1A)	1.28(3)
N(1A)-H(1A1)	0.8600

N(1A)-H(1A2)	0.8600
C(1A)-N(2A)	1.3900
C(1A)-N(6A)	1.3900
N(2A)-C(3A)	1.3900
N(2A)-H(2A)	0.8600
C(3A)-C(4A)	1.3900
C(3A)-H(3A)	0.9300
C(4A)-C(5A)	1.3900
C(4A)-H(4A)	0.9300
C(5A)-N(6A)	1.3900
C(5A)-H(5A)	0.9300
N(1B)-C(1B)	1.34(4)
N(1B)-H(1B1)	0.8600
N(1B)-H(1B2)	0.8600
C(1B)-N(2B)	1.30(4)
C(1B)-N(6B)	1.34(4)
N(2B)-C(3B)	1.34(4)
C(3B)-C(4B)	1.36(5)
C(3B)-H(3B)	0.9300
C(4B)-C(5B)	1.33(5)
C(4B)-H(4B)	0.9300
C(5B)-N(6B)	1.33(4)
C(5B)-H(5B)	0.9300
N(6B)-H(6B)	0.8600
N(1C)-C(1C)	1.34(4)
N(1C)-H(1C1)	0.8600
N(1C)-H(1C2)	0.8600
C(1C)-N(2C)	1.28(4)
C(1C)-N(6C)	1.36(4)
N(2C)-C(3C)	1.36(5)
N(2C)-H(2C)	0.8600
C(3C)-C(4C)	1.29(5)
C(3C)-H(3C)	0.9300
C(4C)-C(5C)	1.36(5)
C(4C)-H(4C)	0.9300
C(5C)-N(6C)	1.33(4)
C(5C)-H(5C)	0.9300
N(1D)-C(1D)	1.28(4)
N(1D)-H(1D1)	0.8600
N(1D)-H(1D2)	0.8600

C(1D)-N(2D)	1.32(4)
C(1D)-N(6D)	1.35(4)
N(2D)-C(3D)	1.33(4)
C(3D)-C(4D)	1.32(5)
C(3D)-H(3D)	0.9300
C(4D)-C(5D)	1.26(5)
C(4D)-H(4D)	0.9300
C(5D)-N(6D)	1.36(4)
C(5D)-H(5D)	0.9300
N(6D)-H(6D)	0.8600
N(1E)-C(1E)	1.32(4)
N(1E)-H(1E1)	0.8600
N(1E)-H(1E2)	0.8600
C(1E)-N(6E)	1.24(4)
C(1E)-N(2E)	1.33(4)
N(2E)-C(3E)	1.32(4)
N(2E)-H(2E)	0.8600
C(3E)-C(4E)	1.25(4)
C(3E)-H(3E)	0.9300
C(4E)-C(5E)	1.36(4)
C(4E)-H(4E)	0.9300
C(5E)-N(6E)	1.28(4)
C(5E)-H(5E)	0.9300
N(1F)-C(1F)	1.30(4)
N(1F)-H(1F1)	0.8600
N(1F)-H(1F2)	0.8600
C(1F)-N(2F)	1.35(4)
C(1F)-N(6F)	1.36(4)
N(2F)-C(3F)	1.30(5)
C(3F)-C(4F)	1.43(5)
C(3F)-H(3F)	0.9300
C(4F)-C(5F)	1.33(4)
C(4F)-H(4F)	0.9300
C(5F)-N(6F)	1.39(5)
C(5F)-H(5F)	0.9300
N(6F)-H(6F)	0.8600
N(1G)-C(1G)	1.31(5)
N(1G)-H(1G1)	0.8600
N(1G)-H(1G2)	0.8600
C(1G)-N(6G)	1.33(5)

C(1G)-N(2G)	1.36(4)
N(2G)-C(3G)	1.32(5)
C(3G)-C(4G)	1.36(6)
C(3G)-H(3G)	0.9300
C(4G)-C(5G)	1.25(6)
C(4G)-H(4G)	0.9300
C(5G)-N(6G)	1.36(5)
C(5G)-H(5G)	0.9300
N(6G)-H(6G)	0.8600
N(1H)-C(1H)	1.30(5)
N(1H)-H(1H1)	0.8600
N(1H)-H(1H2)	0.8600
C(1H)-N(6H)	1.32(5)
C(1H)-N(2H)	1.35(5)
N(2H)-C(3H)	1.30(5)
N(2H)-H(2H)	0.8600
C(3H)-C(4H)	1.37(6)
C(3H)-H(3H)	0.9300
C(4H)-C(5H)	1.32(6)
C(4H)-H(4H)	0.9300
C(5H)-N(6H)	1.30(5)
C(5H)-H(5H)	0.9300
N(1I)-C(1I)	1.32(4)
N(1I)-H(1I1)	0.8600
N(1I)-H(1I2)	0.8600
C(1I)-N(2I)	1.31(4)
C(1I)-N(6I)	1.33(4)
N(2I)-C(3I)	1.33(4)
C(3I)-C(4I)	1.35(4)
C(3I)-H(3I)	0.9300
C(4I)-C(5I)	1.34(4)
C(4I)-H(4I)	0.9300
C(5I)-N(6I)	1.32(4)
C(5I)-H(5I)	0.9300
N(6I)-H(6I)	0.8600
N(1J)-C(1J)	1.29(4)
N(1J)-H(1J1)	0.8600
N(1J)-H(1J2)	0.8600
C(1J)-N(2J)	1.32(4)
C(1J)-N(6J)	1.35(3)

N(2J)-C(3J)	1.29(4)
N(2J)-H(2J)	0.8600
C(3J)-C(4J)	1.38(4)
C(3J)-H(3J)	0.9300
C(4J)-C(5J)	1.39(4)
C(4J)-H(4J)	0.9300
C(5J)-N(6J)	1.29(4)
C(5J)-H(5J)	0.9300
N(1K)-C(1K)	1.28(4)
N(1K)-H(1K1)	0.8600
N(1K)-H(1K2)	0.8600
C(1K)-N(2K)	1.28(4)
C(1K)-N(6K)	1.37(4)
N(2K)-C(3K)	1.29(4)
C(3K)-C(4K)	1.37(4)
C(3K)-H(3K)	0.9300
C(4K)-C(5K)	1.33(4)
C(4K)-H(4K)	0.9300
C(5K)-N(6K)	1.33(4)
C(5K)-H(5K)	0.9300
N(6K)-H(6K)	0.8600
N(1L)-C(1L)	1.38(5)
N(1L)-H(1L1)	0.8600
N(1L)-H(1L2)	0.8600
C(1L)-N(2L)	1.28(5)
C(1L)-N(6L)	1.31(4)
N(2L)-C(3L)	1.39(5)
N(2L)-H(2L)	0.8600
C(3L)-C(4L)	1.24(5)
C(3L)-H(3L)	0.9300
C(4L)-C(5L)	1.38(5)
C(4L)-H(4L)	0.9300
C(5L)-N(6L)	1.32(4)
C(5L)-H(5L)	0.9300
Cl(5)-Bi(1)-Cl(4)	93.1(3)
Cl(5)-Bi(1)-Cl(6)	86.7(3)
Cl(4)-Bi(1)-Cl(6)	86.3(3)
Cl(5)-Bi(1)-Cl(2)	91.5(3)
Cl(4)-Bi(1)-Cl(2)	92.2(3)

Cl(6)-Bi(1)-Cl(2)	177.6(3)
Cl(5)-Bi(1)-Cl(3)	91.9(3)
Cl(4)-Bi(1)-Cl(3)	174.4(3)
Cl(6)-Bi(1)-Cl(3)	96.5(3)
Cl(2)-Bi(1)-Cl(3)	85.1(3)
Cl(5)-Bi(1)-Cl(1)	177.7(3)
Cl(4)-Bi(1)-Cl(1)	89.2(3)
Cl(6)-Bi(1)-Cl(1)	93.4(3)
Cl(2)-Bi(1)-Cl(1)	88.5(3)
Cl(3)-Bi(1)-Cl(1)	85.8(3)
Cl(8)-Bi(2)-Cl(10)	88.9(3)
Cl(8)-Bi(2)-Cl(12)	97.0(3)
Cl(10)-Bi(2)-Cl(12)	89.3(3)
Cl(8)-Bi(2)-Cl(11)	90.0(3)
Cl(10)-Bi(2)-Cl(11)	96.1(3)
Cl(12)-Bi(2)-Cl(11)	171.3(4)
Cl(8)-Bi(2)-Cl(9)	89.7(3)
Cl(10)-Bi(2)-Cl(9)	174.6(3)
Cl(12)-Bi(2)-Cl(9)	85.7(3)
Cl(11)-Bi(2)-Cl(9)	89.2(3)
Cl(8)-Bi(2)-Cl(7)	172.0(3)
Cl(10)-Bi(2)-Cl(7)	84.4(3)
Cl(12)-Bi(2)-Cl(7)	87.4(3)
Cl(11)-Bi(2)-Cl(7)	86.4(3)
Cl(9)-Bi(2)-Cl(7)	97.4(3)
Cl(13)-Bi(3)-Cl(17)	89.3(3)
Cl(13)-Bi(3)-Cl(14)	88.2(3)
Cl(17)-Bi(3)-Cl(14)	96.3(3)
Cl(13)-Bi(3)-Cl(16)	98.7(3)
Cl(17)-Bi(3)-Cl(16)	88.9(3)
Cl(14)-Bi(3)-Cl(16)	171.4(4)
Cl(13)-Bi(3)-Cl(15)	88.9(3)
Cl(17)-Bi(3)-Cl(15)	175.7(3)
Cl(14)-Bi(3)-Cl(15)	87.6(3)
Cl(16)-Bi(3)-Cl(15)	87.5(3)
Cl(13)-Bi(3)-Cl(22)	171.5(3)
Cl(17)-Bi(3)-Cl(22)	84.7(3)
Cl(14)-Bi(3)-Cl(22)	86.5(3)
Cl(16)-Bi(3)-Cl(22)	87.2(3)
Cl(15)-Bi(3)-Cl(22)	97.4(3)

Cl(24)-Bi(4)-Cl(18)	88.4(3)
Cl(24)-Bi(4)-Cl(23)	93.3(3)
Cl(18)-Bi(4)-Cl(23)	90.7(3)
Cl(24)-Bi(4)-Cl(19)	91.7(4)
Cl(18)-Bi(4)-Cl(19)	85.5(3)
Cl(23)-Bi(4)-Cl(19)	173.6(3)
Cl(24)-Bi(4)-Cl(21)	87.1(3)
Cl(18)-Bi(4)-Cl(21)	173.4(3)
Cl(23)-Bi(4)-Cl(21)	84.7(3)
Cl(19)-Bi(4)-Cl(21)	99.5(3)
Cl(24)-Bi(4)-Cl(20)	177.0(3)
Cl(18)-Bi(4)-Cl(20)	90.2(3)
Cl(23)-Bi(4)-Cl(20)	89.3(3)
Cl(19)-Bi(4)-Cl(20)	85.5(4)
Cl(21)-Bi(4)-Cl(20)	94.5(3)
C(1A)-N(1A)-H(1A1)	120.0
C(1A)-N(1A)-H(1A2)	120.0
H(1A1)-N(1A)-H(1A2)	120.0
N(1A)-C(1A)-N(2A)	122(2)
N(1A)-C(1A)-N(6A)	118(2)
N(2A)-C(1A)-N(6A)	120.0
C(1A)-N(2A)-C(3A)	120.0
C(1A)-N(2A)-H(2A)	120.0
C(3A)-N(2A)-H(2A)	120.0
N(2A)-C(3A)-C(4A)	120.0
N(2A)-C(3A)-H(3A)	120.0
C(4A)-C(3A)-H(3A)	120.0
C(5A)-C(4A)-C(3A)	120.0
C(5A)-C(4A)-H(4A)	120.0
C(3A)-C(4A)-H(4A)	120.0
N(6A)-C(5A)-C(4A)	120.0
N(6A)-C(5A)-H(5A)	120.0
C(4A)-C(5A)-H(5A)	120.0
C(5A)-N(6A)-C(1A)	120.0
C(1B)-N(1B)-H(1B1)	120.0
C(1B)-N(1B)-H(1B2)	120.0
H(1B1)-N(1B)-H(1B2)	120.0
N(2B)-C(1B)-N(6B)	119(3)
N(2B)-C(1B)-N(1B)	120(3)
N(6B)-C(1B)-N(1B)	121(3)

C(1B)-N(2B)-C(3B)	116(3)
N(2B)-C(3B)-C(4B)	125(3)
N(2B)-C(3B)-H(3B)	117.4
C(4B)-C(3B)-H(3B)	117.4
C(5B)-C(4B)-C(3B)	118(3)
C(5B)-C(4B)-H(4B)	121.2
C(3B)-C(4B)-H(4B)	121.2
C(4B)-C(5B)-N(6B)	116(3)
C(4B)-C(5B)-H(5B)	121.9
N(6B)-C(5B)-H(5B)	121.9
C(5B)-N(6B)-C(1B)	125(3)
C(5B)-N(6B)-H(6B)	117.3
C(1B)-N(6B)-H(6B)	117.3
C(1C)-N(1C)-H(1C1)	120.0
C(1C)-N(1C)-H(1C2)	120.0
H(1C1)-N(1C)-H(1C2)	120.0
N(2C)-C(1C)-N(1C)	123(3)
N(2C)-C(1C)-N(6C)	122(3)
N(1C)-C(1C)-N(6C)	115(4)
C(1C)-N(2C)-C(3C)	123(3)
C(1C)-N(2C)-H(2C)	118.5
C(3C)-N(2C)-H(2C)	118.5
C(4C)-C(3C)-N(2C)	118(4)
C(4C)-C(3C)-H(3C)	121.2
N(2C)-C(3C)-H(3C)	121.2
C(3C)-C(4C)-C(5C)	118(4)
C(3C)-C(4C)-H(4C)	120.8
C(5C)-C(4C)-H(4C)	120.8
N(6C)-C(5C)-C(4C)	125(3)
N(6C)-C(5C)-H(5C)	117.4
C(4C)-C(5C)-H(5C)	117.4
C(5C)-N(6C)-C(1C)	113(3)
C(1D)-N(1D)-H(1D1)	120.0
C(1D)-N(1D)-H(1D2)	120.0
H(1D1)-N(1D)-H(1D2)	120.0
N(1D)-C(1D)-N(2D)	120(3)
N(1D)-C(1D)-N(6D)	122(3)
N(2D)-C(1D)-N(6D)	117(3)
C(1D)-N(2D)-C(3D)	117(3)
C(4D)-C(3D)-N(2D)	128(4)

C(4D)-C(3D)-H(3D)	116.2
N(2D)-C(3D)-H(3D)	116.2
C(5D)-C(4D)-C(3D)	114(3)
C(5D)-C(4D)-H(4D)	123.1
C(3D)-C(4D)-H(4D)	123.1
C(4D)-C(5D)-N(6D)	123(4)
C(4D)-C(5D)-H(5D)	118.5
N(6D)-C(5D)-H(5D)	118.5
C(1D)-N(6D)-C(5D)	121(3)
C(1D)-N(6D)-H(6D)	119.7
C(5D)-N(6D)-H(6D)	119.7
C(1E)-N(1E)-H(1E1)	120.0
C(1E)-N(1E)-H(1E2)	120.0
H(1E1)-N(1E)-H(1E2)	120.0
N(6E)-C(1E)-N(1E)	122(3)
N(6E)-C(1E)-N(2E)	123(3)
N(1E)-C(1E)-N(2E)	116(3)
C(3E)-N(2E)-C(1E)	120(3)
C(3E)-N(2E)-H(2E)	120.1
C(1E)-N(2E)-H(2E)	120.0
C(4E)-C(3E)-N(2E)	121(3)
C(4E)-C(3E)-H(3E)	119.7
N(2E)-C(3E)-H(3E)	119.7
C(3E)-C(4E)-C(5E)	115(3)
C(3E)-C(4E)-H(4E)	122.4
C(5E)-C(4E)-H(4E)	122.4
N(6E)-C(5E)-C(4E)	126(3)
N(6E)-C(5E)-H(5E)	116.8
C(4E)-C(5E)-H(5E)	116.8
C(1E)-N(6E)-C(5E)	115(3)
C(1F)-N(1F)-H(1F1)	120.0
C(1F)-N(1F)-H(1F2)	120.0
H(1F1)-N(1F)-H(1F2)	120.0
N(1F)-C(1F)-N(2F)	119(3)
N(1F)-C(1F)-N(6F)	123(3)
N(2F)-C(1F)-N(6F)	118(3)
C(3F)-N(2F)-C(1F)	116(3)
N(2F)-C(3F)-C(4F)	130(3)
N(2F)-C(3F)-H(3F)	115.2
C(4F)-C(3F)-H(3F)	115.2

C(5F)-C(4F)-C(3F)	111(4)
C(5F)-C(4F)-H(4F)	124.4
C(3F)-C(4F)-H(4F)	124.4
C(4F)-C(5F)-N(6F)	122(3)
C(4F)-C(5F)-H(5F)	119.1
N(6F)-C(5F)-H(5F)	119.1
C(1F)-N(6F)-C(5F)	123(2)
C(1F)-N(6F)-H(6F)	118.7
C(5F)-N(6F)-H(6F)	118.7
C(1G)-N(1G)-H(1G1)	120.0
C(1G)-N(1G)-H(1G2)	120.0
H(1G1)-N(1G)-H(1G2)	120.0
N(1G)-C(1G)-N(6G)	128(4)
N(1G)-C(1G)-N(2G)	113(4)
N(6G)-C(1G)-N(2G)	119(3)
C(3G)-N(2G)-C(1G)	111(4)
N(2G)-C(3G)-C(4G)	133(4)
N(2G)-C(3G)-H(3G)	113.3
C(4G)-C(3G)-H(3G)	113.3
C(5G)-C(4G)-C(3G)	111(4)
C(5G)-C(4G)-H(4G)	124.7
C(3G)-C(4G)-H(4G)	124.7
C(4G)-C(5G)-N(6G)	124(4)
C(4G)-C(5G)-H(5G)	118.1
N(6G)-C(5G)-H(5G)	118.1
C(1G)-N(6G)-C(5G)	122(3)
C(1G)-N(6G)-H(6G)	119.2
C(5G)-N(6G)-H(6G)	119.2
C(1H)-N(1H)-H(1H1)	120.0
C(1H)-N(1H)-H(1H2)	120.0
H(1H1)-N(1H)-H(1H2)	120.0
N(1H)-C(1H)-N(6H)	119(4)
N(1H)-C(1H)-N(2H)	123(4)
N(6H)-C(1H)-N(2H)	118(4)
C(3H)-N(2H)-C(1H)	127(4)
C(3H)-N(2H)-H(2H)	116.5
C(1H)-N(2H)-H(2H)	116.5
N(2H)-C(3H)-C(4H)	114(4)
N(2H)-C(3H)-H(3H)	123.0
C(4H)-C(3H)-H(3H)	123.0

C(5H)-C(4H)-C(3H)	118(4)
C(5H)-C(4H)-H(4H)	121.0
C(3H)-C(4H)-H(4H)	121.0
N(6H)-C(5H)-C(4H)	127(4)
N(6H)-C(5H)-H(5H)	116.3
C(4H)-C(5H)-H(5H)	116.3
C(5H)-N(6H)-C(1H)	116(4)
C(1I)-N(1I)-H(1I1)	120.0
C(1I)-N(1I)-H(1I2)	120.0
H(1I1)-N(1I)-H(1I2)	120.0
N(2I)-C(1I)-N(1I)	117(4)
N(2I)-C(1I)-N(6I)	124(3)
N(1I)-C(1I)-N(6I)	119(3)
C(1I)-N(2I)-C(3I)	116(3)
N(2I)-C(3I)-C(4I)	124(3)
N(2I)-C(3I)-H(3I)	118.1
C(4I)-C(3I)-H(3I)	118.1
C(5I)-C(4I)-C(3I)	117(3)
C(5I)-C(4I)-H(4I)	121.4
C(3I)-C(4I)-H(4I)	121.4
N(6I)-C(5I)-C(4I)	120(3)
N(6I)-C(5I)-H(5I)	119.9
C(4I)-C(5I)-H(5I)	119.9
C(5I)-N(6I)-C(1I)	119(3)
C(5I)-N(6I)-H(6I)	120.3
C(1I)-N(6I)-H(6I)	120.3
C(1J)-N(1J)-H(1J1)	120.0
C(1J)-N(1J)-H(1J2)	120.0
H(1J1)-N(1J)-H(1J2)	120.0
N(1J)-C(1J)-N(2J)	119(3)
N(1J)-C(1J)-N(6J)	118(3)
N(2J)-C(1J)-N(6J)	124(3)
C(3J)-N(2J)-C(1J)	121(3)
C(3J)-N(2J)-H(2J)	119.6
C(1J)-N(2J)-H(2J)	119.6
N(2J)-C(3J)-C(4J)	121(3)
N(2J)-C(3J)-H(3J)	119.7
C(4J)-C(3J)-H(3J)	119.7
C(3J)-C(4J)-C(5J)	114(3)
C(3J)-C(4J)-H(4J)	122.9

C(5J)-C(4J)-H(4J)	122.9
N(6J)-C(5J)-C(4J)	126(3)
N(6J)-C(5J)-H(5J)	116.8
C(4J)-C(5J)-H(5J)	116.8
C(5J)-N(6J)-C(1J)	114(3)
C(1K)-N(1K)-H(1K1)	120.0
C(1K)-N(1K)-H(1K2)	120.0
H(1K1)-N(1K)-H(1K2)	120.0
N(2K)-C(1K)-N(1K)	124(3)
N(2K)-C(1K)-N(6K)	121(3)
N(1K)-C(1K)-N(6K)	115(3)
C(1K)-N(2K)-C(3K)	118(3)
N(2K)-C(3K)-C(4K)	125(3)
N(2K)-C(3K)-H(3K)	117.3
C(4K)-C(3K)-H(3K)	117.3
C(5K)-C(4K)-C(3K)	116(3)
C(5K)-C(4K)-H(4K)	122.0
C(3K)-C(4K)-H(4K)	122.0
C(4K)-C(5K)-N(6K)	119(3)
C(4K)-C(5K)-H(5K)	120.3
N(6K)-C(5K)-H(5K)	120.3
C(5K)-N(6K)-C(1K)	120(2)
C(5K)-N(6K)-H(6K)	119.8
C(1K)-N(6K)-H(6K)	119.8
C(1L)-N(1L)-H(1L1)	120.0
C(1L)-N(1L)-H(1L2)	120.0
H(1L1)-N(1L)-H(1L2)	120.0
N(2L)-C(1L)-N(6L)	124(4)
N(2L)-C(1L)-N(1L)	122(3)
N(6L)-C(1L)-N(1L)	114(4)
C(1L)-N(2L)-C(3L)	119(3)
C(1L)-N(2L)-H(2L)	120.7
C(3L)-N(2L)-H(2L)	120.7
C(4L)-C(3L)-N(2L)	122(4)
C(4L)-C(3L)-H(3L)	119.0
N(2L)-C(3L)-H(3L)	119.0
C(3L)-C(4L)-C(5L)	116(4)
C(3L)-C(4L)-H(4L)	122.2
C(5L)-C(4L)-H(4L)	122.2
N(6L)-C(5L)-C(4L)	125(3)

N(6L)-C(5L)-H(5L)	117.3
C(4L)-C(5L)-H(5L)	117.3
C(1L)-N(6L)-C(5L)	114(3)

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**Table S6** Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **2**.

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Bi(1)-Cl(3)	2.531(3)
Bi(1)-Cl(5)	2.577(3)
Bi(1)-Cl(4)	2.685(3)
Bi(1)-Cl(2)	2.792(3)
Bi(1)-Cl(1)	2.844(3)
Bi(1)-Cl(2)#1	2.934(2)
Cl(2)-Bi(1)#1	2.934(2)
N(1A)-C(1A)	1.306(14)
N(1A)-H(1A1)	0.8600
N(1A)-H(1A2)	0.8600
N(2A)-C(2A)	1.334(15)
N(2A)-C(1A)	1.337(14)
N(2A)-H(2A)	0.8600
N(3A)-C(4A)	1.324(13)
N(3A)-C(1A)	1.342(13)
C(2A)-C(3A)	1.346(15)
C(2A)-H(2A)	0.9300
C(3A)-C(4A)	1.367(16)
C(3A)-H(3A)	0.9300
C(4A)-H(4A)	0.9300
N(1B)-C(1B)	1.302(14)
N(1B)-H(1B1)	0.8600
N(1B)-H(1B2)	0.8600
N(2B)-C(2B)	1.308(14)
N(2B)-C(1B)	1.352(13)
N(3B)-C(4B)	1.335(14)
N(3B)-C(1B)	1.364(14)
N(3B)-H(3B)	0.8600
C(2B)-C(3B)	1.383(16)
C(2B)-H(2B)	0.9300
C(3B)-C(4B)	1.354(17)
C(3B)-H(3B)	0.9300

C(4B)-H(4B)	0.9300
Cl(3)-Bi(1)-Cl(5)	91.80(12)
Cl(3)-Bi(1)-Cl(4)	91.98(10)
Cl(5)-Bi(1)-Cl(4)	91.66(11)
Cl(3)-Bi(1)-Cl(2)	86.66(8)
Cl(5)-Bi(1)-Cl(2)	92.39(10)
Cl(4)-Bi(1)-Cl(2)	175.77(9)
Cl(3)-Bi(1)-Cl(1)	92.55(10)
Cl(5)-Bi(1)-Cl(1)	175.08(10)
Cl(4)-Bi(1)-Cl(1)	90.49(9)
Cl(2)-Bi(1)-Cl(1)	85.58(8)
Cl(3)-Bi(1)-Cl(2)#1	171.82(8)
Cl(5)-Bi(1)-Cl(2)#1	89.78(10)
Cl(4)-Bi(1)-Cl(2)#1	96.00(8)
Cl(2)-Bi(1)-Cl(2)#1	85.26(7)
Cl(1)-Bi(1)-Cl(2)#1	85.59(8)
Bi(1)-Cl(2)-Bi(1)#1	94.74(7)
C(1A)-N(1A)-H(1A1)	120.0
C(1A)-N(1A)-H(1A2)	120.0
H(1A1)-N(1A)-H(1A2)	120.0
C(2A)-N(2A)-C(1A)	122.3(9)
C(2A)-N(2A)-H(2A)	118.9
C(1A)-N(2A)-H(2A)	118.9
C(4A)-N(3A)-C(1A)	116.1(9)
N(1A)-C(1A)-N(2A)	120.4(10)
N(1A)-C(1A)-N(3A)	118.9(10)
N(2A)-C(1A)-N(3A)	120.7(10)
N(2A)-C(2A)-C(3A)	119.1(10)
N(2A)-C(2A)-H(2A)	120.5
C(3A)-C(2A)-H(2A)	120.5
C(2A)-C(3A)-C(4A)	116.7(11)
C(2A)-C(3A)-H(3A)	121.7
C(4A)-C(3A)-H(3A)	121.7
N(3A)-C(4A)-C(3A)	125.1(10)
N(3A)-C(4A)-H(4A)	117.5
C(3A)-C(4A)-H(4A)	117.5
C(1B)-N(1B)-H(1B1)	120.0
C(1B)-N(1B)-H(1B2)	120.0
H(1B1)-N(1B)-H(1B2)	120.0

C(2B)-N(2B)-C(1B)	116.9(10)
C(4B)-N(3B)-C(1B)	122.1(9)
C(4B)-N(3B)-H(3B)	119.0
C(1B)-N(3B)-H(3B)	119.0
N(1B)-C(1B)-N(2B)	119.5(10)
N(1B)-C(1B)-N(3B)	120.2(10)
N(2B)-C(1B)-N(3B)	120.2(9)
N(2B)-C(2B)-C(3B)	124.8(11)
N(2B)-C(2B)-H(2B)	117.6
C(3B)-C(2B)-H(2B)	117.6
C(4B)-C(3B)-C(2B)	117.3(11)
C(4B)-C(3B)-H(3B)	121.4
C(2B)-C(3B)-H(3B)	121.4
N(3B)-C(4B)-C(3B)	118.7(11)
N(3B)-C(4B)-H(4B)	120.6
C(3B)-C(4B)-H(4B)	120.6

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Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+2

**Table S7** Hydrogen bonds for **1** [ $\text{\AA}$  and  $^\circ$ ].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
N(1A)-H(1A1)...Cl(7)	0.86	2.71	3.44(3)	143.5
N(1A)-H(1A2)...Cl(4)#1	0.86	2.53	3.37(3)	167.6
N(2A)-H(2A)...Cl(7)	0.86	2.48	3.233(19)	147.2
C(3A)-H(3A)...Cl(5)#2	0.93	2.59	3.32(2)	135.7
C(3A)-H(3A)...Cl(12)	0.93	2.91	3.60(2)	132.5
C(5A)-H(5A)...Cl(7)#3	0.93	2.92	3.69(2)	141.2
C(5A)-H(5A)...Cl(10)#4	0.93	2.78	3.48(2)	133.3
N(1B)-H(1B1)...Cl(13)	0.86	2.63	3.42(3)	153.5
N(1B)-H(1B2)...Cl(1)	0.86	2.76	3.41(4)	132.6
C(3B)-H(3B)...Cl(1)#5	0.93	2.89	3.60(3)	134.9
C(4B)-H(4B)...Cl(15)#5	0.93	2.97	3.53(3)	120.4
C(5B)-H(5B)...Cl(2)	0.93	2.87	3.49(5)	125.9
C(5B)-H(5B)...Cl(15)#5	0.93	2.86	3.48(3)	125.3
N(6B)-H(6B)...Cl(1)	0.86	2.94	3.57(3)	132.0
N(6B)-H(6B)...Cl(2)	0.86	2.96	3.55(3)	127.4

N(6B)-H(6B)...Cl(3)	0.86	2.95	3.64(3)	138.6
N(1C)-H(1C1)...Cl(18)#6	0.86	2.58	3.18(3)	127.9
N(1C)-H(1C2)...N(2D)	0.86	2.33	3.19(5)	177.5
N(2C)-H(2C)...Cl(9)	0.86	2.32	3.18(3)	176.2
C(4C)-H(4C)...N(6A)#4	0.93	2.64	3.49(7)	152.2
C(5C)-H(5C)...Cl(4)#5	0.93	2.77	3.36(3)	122.4
N(1D)-H(1D1)...N(6C)	0.86	2.27	3.13(4)	177.2
N(1D)-H(1D2)...Cl(2)#5	0.86	2.58	3.23(3)	133.8
C(3D)-H(3D)...Cl(23)#6	0.93	2.84	3.42(3)	122.0
C(4D)-H(4D)...N(6E)#6	0.93	2.69	3.56(4)	158.0
N(6D)-H(6D)...Cl(15)#7	0.86	2.27	3.12(3)	169.7
N(1E)-H(1E2)...Cl(22)	0.86	2.66	3.39(3)	144.2
N(1E)-H(1E1)...Cl(23)	0.86	2.49	3.34(3)	170.9
N(2E)-H(2E)...Cl(22)	0.86	2.63	3.35(3)	142.4
C(3E)-H(3E)...Cl(16)	0.93	2.91	3.62(4)	134.7
C(3E)-H(3E)...Cl(24)#6	0.93	2.63	3.36(3)	135.5
C(5E)-H(5E)...Cl(17)#8	0.93	2.81	3.57(3)	139.3
N(1F)-H(1F2)...Cl(11)#9	0.86	2.62	3.17(3)	122.2
N(1F)-H(1F2)...Cl(20)	0.86	2.80	3.47(3)	136.0
N(1F)-H(1F1)...N(2K)	0.86	2.26	3.11(4)	171.2
C(3F)-H(3F)...Cl(14)	0.93	2.90	3.71(3)	146.6
C(3F)-H(3F)...Cl(17)	0.93	2.96	3.58(4)	125.3
C(4F)-H(4F)...Cl(17)	0.93	2.86	3.47(4)	124.8
C(5F)-H(5F)...Cl(23)	0.93	2.99	3.44(3)	111.8
N(6F)-H(6F)...Cl(20)	0.86	2.37	3.14(3)	149.9
N(1G)-H(1G1)...Cl(6)#10	0.86	2.52	3.20(3)	136.9
N(1G)-H(1G2)...N(6L)	0.86	2.36	3.22(4)	177.4
C(3G)-H(3G)...Cl(19)	0.93	2.76	3.49(4)	136.2
C(5G)-H(5G)...Cl(9)#11	0.93	2.90	3.81(5)	168.2
N(6G)-H(6G)...Cl(7)#11	0.86	2.33	3.19(3)	174.3
N(1H)-H(1H1)...Cl(9)#8	0.86	2.52	3.26(4)	145.2
N(1H)-H(1H2)...Cl(18)	0.86	2.40	3.21(5)	157.4
N(2H)-H(2H)...Cl(20)	0.86	2.45	3.16(3)	140.3
C(3H)-H(3H)...Cl(11)#9	0.93	2.71	3.63(5)	173.5
C(5H)-H(5H)...Cl(19)#12	0.93	2.98	3.75(5)	140.8
N(1I)-H(1I1)...N(6J)	0.86	2.21	3.07(4)	176.5
N(1I)-H(1I2)...Cl(5)#13	0.86	2.67	3.37(3)	140.0
N(1I)-H(1I2)...Cl(12)#8	0.86	2.77	3.33(3)	124.4
C(3I)-H(3I)...Cl(13)#8	0.93	2.80	3.49(3)	131.2
C(4I)-H(4I)...Cl(13)#8	0.93	2.95	3.54(3)	122.0

C(5I)-H(5I)...Cl(3)#13	0.93	2.95	3.49(3)	118.6
N(6I)-H(6I)...Cl(4)#14	0.86	2.92	3.43(3)	120.2
N(6I)-H(6I)...Cl(5)#13	0.86	2.40	3.16(3)	148.0
N(1J)-H(1J1)...Cl(16)#8	0.86	2.62	3.24(3)	129.4
N(1J)-H(1J1)...Cl(24)	0.86	2.82	3.49(3)	136.4
N(1J)-H(1J2)...N(2I)	0.86	2.26	3.12(4)	174.0
N(2J)-H(2J)...Cl(23)#10	0.86	2.98	3.46(3)	116.6
N(2J)-H(2J)...Cl(24)	0.86	2.35	3.14(3)	151.5
C(4J)-H(4J)...Cl(8)#8	0.93	2.84	3.47(3)	126.2
C(5J)-H(5J)...Cl(8)#8	0.93	2.91	3.55(3)	126.4
N(1K)-H(1K1)...N(2F)	0.86	2.26	3.11(4)	173.1
N(1K)-H(1K2)...Cl(1)	0.86	2.70	3.44(3)	145.0
N(1K)-H(1K2)...Cl(14)	0.86	2.64	3.15(3)	119.2
C(3K)-H(3K)...Cl(10)#9	0.93	2.90	3.54(3)	127.7
C(3K)-H(3K)...Cl(11)#9	0.93	2.89	3.69(3)	145.9
C(4K)-H(4K)...Cl(10)#9	0.93	2.89	3.51(3)	124.7
C(5K)-H(5K)...Cl(4)	0.93	2.86	3.38(3)	116.4
N(6K)-H(6K)...Cl(1)	0.86	2.43	3.20(3)	150.0
N(1L)-H(1L1)...Cl(21)	0.86	2.32	3.11(3)	152.6
N(1L)-H(1L2)...N(2G)	0.86	2.21	3.06(5)	169.1
N(2L)-H(2L)...Cl(22)	0.86	2.35	3.18(3)	160.3
C(5L)-H(5L)...Cl(3)#10	0.93	2.76	3.43(4)	130.3

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z-1 #2 -x+2,y+1/2,-z+1 #3 -x+2,y+1/2,-z  
 #4 -x+2,y-1/2,-z #5 -x+2,y-1/2,-z+1 #6 -x+1,y-1/2,-z+1  
 #7 x,y-1,z #8 -x+1,y+1/2,-z+1 #9 x,y,z+1  
 #10 x,y+1,z #11 x,y+1,z+1 #12 -x+1,y-1/2,-z+2  
 #13 x-1,y+1,z #14 x-1,y,z

**Table S8** Hydrogen bonds for **2** [ $\text{\AA}$  and  $^\circ$ ].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
N(1A)-H(1A1)...Cl(1)#2	0.86	2.57	3.229(10)	134.0
N(1A)-H(1A2)...N(2B)	0.86	2.16	3.010(14)	171.0
N(2A)-H(2A)...Cl(1)	0.86	2.24	3.089(9)	171.1
C(2A)-H(2A)...Cl(5)#3	0.93	2.99	3.613(12)	126.1
C(4A)-H(4A)...Cl(2)#4	0.93	2.83	3.647(11)	146.5
C(4A)-H(4A)...Cl(3)#4	0.93	2.86	3.550(11)	131.6

N(1B)-H(1B1)...N(3A)	0.86	2.24	3.094(14)	170.5
N(1B)-H(1B2)...Cl(2)#4	0.86	2.83	3.337(10)	119.6
N(1B)-H(1B2)...Cl(4)#5	0.86	2.82	3.534(11)	141.8
N(3B)-H(3B)...Cl(4)#5	0.86	2.40	3.204(10)	155.1
C(3B)-H(3B)...Cl(3)#6	0.93	2.83	3.452(12)	125.1
C(4B)-H(4B)...Cl(3)#6	0.93	2.90	3.487(12)	122.1

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Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+2 #2 -x+1,-y+1,-z+2 #3 x-1,y,z

#4 -x,-y,-z+1 #5 x-1,y,z-1 #6 -x+1,-y+1,-z+1

## Bioactivity tests

MTT-assay method<sup>1,2</sup> is based on the ability of dehydrogenases of living cells to convert 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl-2H-tetrazolium bromide (MTT) into insoluble formazan crystals, which after an extraction with isopropanol was determined using a Microplate Reader 550 (Bio'Rad) instrument at  $\lambda = 550$  nm. The normal lymphocytes and Jurkat leukemic cell line were used.

## References

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2. M. A. Orlova, E. Yu. Osipova and D. A. Roumiantsev, *Br. J. Med. Med. Res.*, 2012, **2**, 21.