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Supporting information for article:

Understanding distortions of inorganic substructures in chloridobismuthates(III)

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Supporting information

Table S1 Selected crystal data and structure determination summary for **1** at 295 and 100 K as well as for **2** at 295 K.

	1	**1**	**2**
Temperature (K)	295(2)	100.0(1)	295(2)
Formula	$C_6H_{21}BiCl_6N_3$	$C_6H_{21}BiCl_6N_3$	$C_4H_{14}BiCl_5N_2$
M_r	556.94	556.94	476.40
Crystal size (mm)	0.25 × 0.16 × 0.09	0.25 × 0.16 × 0.09	0.35 × 0.23 × 0.13
Crystal system	Monoclinic	Monoclinic	Orthorhombic
Space group, Z	$C2/c$, 8	$C2/c$, 8	$P2_12_12_1$, 4
a (Å)	27.8842(4)	27.5447(3)	7.60312(9)
b (Å)	10.19431(13)	10.14187(11)	12.50404(14)
c (Å)	12.45639(17)	12.38379(14)	13.63023(15)
α (º)	90	90	90
β (º)	102.9110(14)	102.9055(12)	90
γ (º)	90	90	90
V (Å^3)	3451.34(8)	3372.08(7)	1295.82(3)
ρ (g/cm^3)	2.144	2.194	2.442
μ (mm^{-1})	11.128	11.390	14.596
θ range (º)	3.00 - 26.00	3.04 - 26.00	3.07 - 26.00
Index ranges	$-34 \le h \le 34$	$-33 \le h \le 33$	$-9 \le h \le 5$
	$-9 \le k \le 12$	$-8 \le k \le 12$	$-15 \le k \le 15$
	$-15 \le l \le 15$	$-15 \le l \le 15$	$-16 \le l \le 16$
Reflns collected	11329	10977	8742
R_{int}	0.0166	0.0144	0.0121
Data [$I > 2\sigma(I)$]	3130	3182	2514
Data/parameters	3386/189	3301/188	2545/113
GOF on F^2	1.046	1.100	1.143
R_1 [$F^2 > 2\sigma(F^2)$]	0.0156	0.0156	0.0100
R_1 (all data)	0.0179	0.0165	0.0104
wR_2 (all data)	0.0368	0.0373	0.0237
Lrgst diff peak (e/Å^3)	0.628	0.922	0.464
Lrgst diff hole (e/Å^3)	–0.450	–0.882	–0.313
CCDC number	2067265	2067266	2067267

Table S2 Selected crystal data and structure determination summary for **3** and **4** at 295 K.

	3	**4**
Temperature (K)	295(2)	295(2)
Formula	$C_{15}H_{42}Bi_2Cl_9N_9$	$C_{10}H_{28}Bi_2Cl_8N_6$
M_r	1085.59	933.94
Crystal size (mm)	0.22 × 0.20 × 0.19	0.31 × 0.22 × 0.06
Crystal system	Monoclinic	Triclinic
Space group, Z	$P2_1/n$, 4	$P\bar{1}$; 2
a (Å)	10.57031(17)	7.7179(3)
b (Å)	29.2063(4)	10.5660(5)
c (Å)	12.04367(19)	18.0362(7)
α (º)	90	95.585(3)
β (º)	106.6342(17)	91.008(3)
γ (º)	90	110.965(4)
V (Å^3)	3562.52(10)	1364.74(11)
ρ (g/cm^3)	2.024	2.273
μ (mm^{-1})	10.563	13.669
θ range (º)	3.08 - 26.00	3.00 - 26.00
Index ranges	$-13 \le h \le 13$	$-9 \le h \le 6$
	$-36 \le k \le 36$	$-13 \le k \le 13$
	$-14 \le l \le 11$	$-22 \le l \le 22$
Reflns collected	23916	9281
R_{int}	0.0230	0.0302
Data [$I > 2\sigma(I)$]	6102	4631
Data/parameters	6979/329	5286/244
GOF on F^2	1.028	1.077
R_1 [$F^2 > 2\sigma(F^2)$]	0.0181	0.0257
R_1 (all data)	0.0239	0.0312
wR_2 (all data)	0.0370	0.0594
Lrgst diff peak (e/Å^3)	0.696	0.686
Lrgst diff hole (e/Å^3)	–0.629	–0.763
CCDC number	2067268	2067269

Table S3 Selected bond lengths (Å) and bond angles (°) for **1** at 295 and 100 K as well as for **2** at 295 K.

	1	**1**		**2**
	295(2)	100.0(1)		295(2)
Bi1–Cl1	2.6597(8)	2.6858(7)	Bi1–Cl1	2.5764(11)
Bi1–Cl2	2.7707(8)	2.7507(7)	Bi1–Cl2	2.8650(11)
Bi1–Cl3	2.7049(8)	2.6906(7)	Bi1–Cl2^{i}	2.8788(11)
Bi1–Cl4	2.6866(8)	2.6939(7)	Bi1–Cl3	2.5735(11)
Bi1–Cl5	2.7045(8)	2.6985(7)	Bi1–Cl4	2.6853(10)
Bi1–Cl6	2.7047(10)	2.7120(9)	Bi1–Cl5	2.7085(11)
Cl1–Bi1–Cl2	176.27(3)	175.87(2)	Cl1–Bi1–Cl2	174.69(4)
Cl1–Bi1–Cl3	89.82(3)	89.43(2)	Cl1–Bi1–Cl2^{i}	88.33(4)
Cl1–Bi1–Cl4	88.66(3)	88.79(2)	Cl1–Bi1–Cl3	92.12(4)
Cl1–Bi1–Cl5	89.33(3)	89.55(2)	Cl1–Bi1–Cl4	89.12(4)
Cl1–Bi1–Cl6	89.43(4)	88.92(3)	Cl1–Bi1–Cl5	94.18(4)
Cl2–Bi1–Cl3	87.37(2)	86.97(2)	Cl2–Bi1–Cl2^{i}	87.077(12)
Cl2–Bi1–Cl4	94.28(2)	94.91(2)	Cl2–Bi1–Cl3	92.42(4)
Cl2–Bi1–Cl5	88.19(3)	88.38(2)	Cl2–Bi1–Cl4	88.27(4)
Cl2–Bi1–Cl6	92.97(3)	93.06(3)	Cl2–Bi1–Cl5	88.35(4)
Cl3–Bi1–Cl4	176.53(3)	176.20(2)	Cl2^{i}–Bi1–Cl3	178.62(4)
Cl3–Bi1–Cl5	89.14(3)	89.53(2)	Cl2^{i}–Bi1–Cl4	90.40(4)
Cl3–Bi1–Cl6	89.18(3)	89.19(3)	Cl2^{i}–Bi1–Cl5	88.46(4)
Cl4–Bi1–Cl5	93.97(3)	93.82(2)	Cl3–Bi1–Cl4	88.30(4)
Cl4–Bi1–Cl6	87.68(3)	87.41(3)	Cl3–Bi1–Cl5	92.81(4)
Cl5–Bi1–Cl6	177.91(3)	178.02(3)	Cl4–Bi1–Cl5	176.48(4)
N11–C11	1.471(7)	1.478(7)	Bi1–Cl2–Bi1^{ii}	148.62(5)
C11–C12	1.518(8)	1.521(7)	N1–C1	1.470(6)
N12–C12	1.481(8)	1.494(7)	C1–C2	1.483(7)
N12–C13	1.445(9)	1.440(8)	N2–C2	1.510(6)
N12–C14	1.547(11)	1.596(8)	N2–C3	1.485(6)
N21–C21	1.471(4)	1.489(4)	N2–C4	1.486(6)
C21–C22	1.494(5)	1.510(4)	N1–C1–C2	110.4(4)
N221–C22	1.483(5)	1.495(4)	N2–C2–C1	111.0(4)
N221–C23	1.486(6)	1.491(5)	C2–N2–C3	114.9(4)
N221–C24	1.508(6)	1.502(5)	C2–N2–C4	109.2(4)
N222–C22	1.475(8)	1.508(13)	C3–N2–C4	109.9(4)
N222–C23	1.565(9)	1.577(14)		
N222–C24	1.415(9)	1.377(14)		
N11–C11–C12	109.3(5)	108.7(4)		
N12–C12–C11	111.6(5)	110.9(4)		
C12–N12–C13	142.2(6)	141.5(5)		
C12–N12–C14	75.3(5)	73.5(4)		
C13–N12–C14	109.5(6)	107.9(4)		
N21–C21–C22	111.9(3)	110.3(3)		
N221–C22–C21	116.0(3)	113.7(3)		
N222–C22–C21	112.9(4)	111.7(6)		
C22–N221–C23	111.0(4)	111.0(3)		
C22–N221–C24	113.6(4)	113.9(3)		
C22–N222–C23	107.2(6)	105.8(9)		
C22–N222–C24	120.0(7)	121.0(10)		
C23–N221–C24	109.8(4)	109.7(3)		
C23–N222–C24	110.6(6)	111.7(9)		

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

Table S4 Selected bond lengths (Å) and bond angles (°) for **3** and **4** at 295 K.

3				**4**			
295(2)				295(2)			
Bi1–Cl1	2.5301(9)	N11–C11	1.322(4)	Bi1–Cl1	2.4917(13)	N11–C11	1.329(7)
Bi1–Cl2	3.0527(9)	N12–C11	1.310(4)	Bi1–Cl2	3.0826(14)	N12–C11	1.326(7)
Bi1–Cl4	2.5378(9)	N13–C11	1.329(4)	Bi1–Cl3	2.5011(15)	N13–C11	1.319(6)
Bi1–Cl5	2.9754(8)	N12–C12	1.512(5)	Bi1–Cl4	3.0199(15)	N12–C12	1.453(8)
Bi1–Cl7	2.6055(9)	N12–C13	1.457(5)	Bi1–Cl5	2.7033(13)	N12–C13	1.460(7)
Bi1–Cl8	2.8357(9)	N13–C14	1.464(5)	Bi1–Cl6	2.7441(15)	N13–C14	1.442(8)
Bi2–Cl2	2.9797(9)	N13–C15	1.445(4)	Bi2–Cl2^{i}	2.7220(13)	N13–C15	1.458(8)
Bi2–Cl3	2.5534(9)	N21–C21	1.320(4)	Bi2–Cl4	2.7119(14)	N21–C21	1.330(7)
Bi2–Cl5	2.8621(8)	N22–C21	1.331(4)	Bi2–Cl5	2.9925(14)	N22–C21	1.318(7)
Bi2–Cl6	2.6088(8)	N23–C21	1.322(4)	Bi2–Cl6^{i}	2.9010(15)	N23–C21	1.333(7)
Bi2–Cl8	2.8890(9)	N22–C22	1.446(4)	Bi2–Cl7	2.5212(15)	N22–C22	1.450(8)
Bi2–Cl9	2.5704(9)	N22–C23	1.461(4)	Bi2–Cl8	2.5572(14)	N22–C23	1.479(7)
Cl1–Bi1–Cl2	164.13(3)	N23–C24	1.462(5)	Cl1–Bi1–Cl2	166.53(5)	N23–C24	1.461(8)
Cl1–Bi1–Cl4	94.60(3)	N23–C25	1.455(4)	Cl1–Bi1–Cl3	91.12(5)	N23–C25	1.456(8)
Cl1–Bi1–Cl5	89.59(3)	N31–C31	1.320(4)	Cl1–Bi1–Cl4	91.01(5)	N11–C11–N12	119.2(5)
Cl1–Bi1–Cl7	90.67(3)	N32–C31	1.339(4)	Cl1–Bi1–Cl5	89.01(5)	N11–C11–N13	119.1(5)
Cl1–Bi1–Cl8	91.08(3)	N33–C31	1.327(4)	Cl1–Bi1–Cl6	87.39(5)	N12–C11–N13	121.6(6)
Cl2–Bi1–Cl4	97.29(3)	N32–C32	1.458(4)	Cl2–Bi1–Cl3	84.94(5)	C11–N12–C12	122.8(5)
Cl2–Bi1–Cl5	77.74(2)	N32–C33	1.461(4)	Cl2–Bi1–Cl4	95.48(5)	C11–N12–C13	120.5(5)
Cl2–Bi1–Cl7	99.48(3)	N33–C34	1.463(4)	Cl2–Bi1–Cl5	103.72(4)	C11–N13–C14	123.5(5)
Cl2–Bi1–Cl8	77.73(3)	N33–C35	1.467(4)	Cl2–Bi1–Cl6	79.84(4)	C11–N13–C15	121.6(6)
Cl4–Bi1–Cl5	173.61(3)	N11–C11–N12	118.1(4)	Cl3–Bi1–Cl4	168.17(5)	C12–N12–C13	115.6(5)
Cl4–Bi1–Cl7	91.47(3)	N11–C11–N13	120.9(3)	Cl3–Bi1–Cl5	88.43(5)	C14–N13–C15	113.9(5)
Cl4–Bi1–Cl8	93.67(3)	N12–C11–N13	121.1(3)	Cl3–Bi1–Cl6	91.22(6)	N21–C21–N22	119.3(5)
Cl5–Bi1–Cl7	93.31(3)	C11–N12–C12	121.0(3)	Cl4–Bi1–Cl5	79.98(4)	N21–C21–N23	118.7(5)
Cl5–Bi1–Cl8	81.41(2)	C11–N12–C13	121.7(4)	Cl4–Bi1–Cl6	100.50(6)	N22–C21–N23	122.0(5)
Cl7–Bi1–Cl8	174.42(3)	C11–N13–C14	124.9(3)	Cl5–Bi1–Cl6	176.37(5)	C21–N22–C22	122.9(5)
Cl2–Bi2–Cl3	171.77(3)	C11–N13–C15	119.4(3)	Cl2^{I}–Bi2–Cl4	177.58(5)	C21–N22–C23	120.7(5)
Cl2–Bi2–Cl5	80.70(2)	C12–N12–C13	116.1(3)	Cl2^{I}–Bi2–Cl5	102.06(5)	C21–N23–C24	122.8(5)
Cl2–Bi2–Cl6	94.33(3)	C14–N13–C15	114.9(3)	Cl2^{I}–Bi2–Cl6^{i}	83.54(4)	C21–N23–C25	121.5(5)
Cl2–Bi2–Cl8	78.12(3)	N21–C21–N22	119.3(3)	Cl2^{I}–Bi2–Cl7	89.77(5)	C22–N22–C23	115.0(5)
Cl2–Bi2–Cl9	92.05(3)	N21–C21–N23	119.0(3)	Cl2^{I}–Bi2–Cl8	89.78(5)	C24–N23–C25	115.0(5)
Cl3–Bi2–Cl5	94.62(3)	N22–C21–N23	121.7(3)	Cl4–Bi2–Cl5	80.34(4)		
Cl3–Bi2–Cl6	89.63(3)	C21–N22–C22	121.7(3)	Cl4–Bi2–Cl6^{i}	96.85(5)		
Cl3–Bi2–Cl8	94.62(3)	C21–N22–C23	120.5(3)	Cl4–Bi2–Cl7	87.84(5)		
Cl3–Bi2–Cl9	95.12(3)	C21–N23–C24	121.8(3)	Cl4–Bi2–Cl8	89.98(5)		
Cl5–Bi2–Cl6	172.59(3)	C21–N23–C25	122.3(3)	Cl5–Bi2–Cl6^{i}	90.46(6)		
Cl5–Bi2–Cl8	82.48(2)	C22–N22–C23	115.6(3)	Cl5–Bi2–Cl7	168.16(5)		
Cl5–Bi2–Cl9	94.98(3)	C24–N23–C25	114.8(3)	Cl5–Bi2–Cl8	87.43(5)		
Cl6–Bi2–Cl8	91.14(3)	N31–C31–N32	119.4(3)	Cl6^{I}–Bi2–Cl7	90.17(6)		
Cl6–Bi2–Cl9	90.67(3)	N31–C31–N33	119.9(3)	Cl6^{I}–Bi2–Cl8	172.42(5)		
Cl8–Bi2–Cl9	170.11(3)	N32–C31–N33	120.7(3)	Cl7–Bi2–Cl8	93.38(6)		
Bi1–Cl2–Bi2	81.51(2)	C31–N32–C32	121.4(3)	Bi1–Cl2–Bi2^{ii}	96.37(4)		
Bi1–Cl5–Bi2	84.84(2)	C31–N32–C33	120.7(3)	Bi1–Cl4–Bi2	99.03(4)		
Bi1–Cl8–Bi2	86.94(2)	C31–N33–C34	122.3(3)	Bi1–Cl5–Bi2	99.90(4)		
		C31–N33–C35	120.8(3)	Bi1–Cl6–Bi2^{ii}	100.22(5)		
		C32–N32–C33	115.6(3)				
		C34–N33–C35	114.9(3)				

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

Table S5 Hydrogen bonds geometries (Å, °) for **1** at 295 K compared to those commensurate with the sums of the van der Waals radii of respective atoms at 100 K (Bondi, 1964; Nyburg & Faerman, 1985; Batsanov, 2001; Hu *et al.*, 2014).

	D–H	H···A	D···A	D–H···A
		295(2) K		
N11–H113···Cl1^{i}	0.89	2.82	3.628(11)	152
N11–H111···Cl4	0.89	2.83	3.421(14)	125
N11–H111···Cl6^{i}	0.89	2.66	3.013(6)	105
N11–H112···Cl6^{ii}	0.89	2.63	3.474(6)	160
N12–H121···Cl2	0.98	2.18	3.118(5)	160
N21–H213···Cl1^{iii}	0.89	2.35	3.237(3)	171
N21–H212···Cl2^{iv}	0.89	2.36	3.176(3)	152
N21–H211···Cl3^{v}	0.89	2.44	3.183(3)	142
N221–H221···Cl1^{vi}	0.98	2.57	3.379(5)	140
N221–H221···Cl4^{iii}	0.98	2.90	3.471(5)	118
N222–H222···Cl3	0.98	2.19	3.098(11)	154
C11–H114···Cl4^{ii}	0.97	2.81	3.595(6)	139
C11–H114···Cl4^{vii}	0.97	2.83	3.500(7)	127
C11–H115···Cl4	0.97	2.88	3.429(7)	117
C12–H122···Cl2^{vii}	0.97	2.83	3.673(6)	146
C13–H132···Cl6^{vi}	0.96	2.69	3.272(8)	120
C14–H141···Cl6	0.96	2.61	3.489(8)	152
C21–H215···Cl5^{iii}	0.97	2.87	3.667(4)	141
C22–H223···Cl3	0.97	2.84	3.535(3)	130
C22–H224···Cl4^{iii}	0.97	2.83	3.577(3)	134
C23–H232···Cl4^{iii}	0.96	2.88	3.541(4)	127
C24–H242···Cl3^{vi}	0.96	2.65	3.590(4)	166
C24–H243···Cl3	0.96	2.78	3.641(4)	150
		100.0(1) K		
N11–H113···Cl1^{i}	0.89	2.70	3.541(5)	159
N11–H111···Cl4	0.89	2.77	3.392(7)	128
N11–H111···Cl6^{i}	0.89	2.61	2.959(5)	104
N11–H112···Cl6^{ii}	0.89	2.60	3.463(5)	164
N12–H121···Cl2	0.98	2.17	3.093(4)	157
N21–H213···Cl1^{iii}	0.89	2.33	3.216(3)	175
N21–H212···Cl2^{iv}	0.89	2.36	3.161(3)	150
N21–H211···Cl3^{v}	0.89	2.42	3.163(3)	142
N221–H221···Cl1^{vi}	0.98	2.51	3.307(4)	139
N221–H221···Cl4^{iii}	0.98	2.86	3.425(4)	118
N222–H222···Cl3	0.98	2.18	3.079(17)	151
C11–H114···Cl4^{ii}	0.97	2.79	3.584(5)	140
C11–H114···Cl4^{vii}	0.97	2.78	3.451(6)	127
C11–H115···Cl4	0.97	2.83	3.383(6)	117
C12–H122···Cl2^{vii}	0.97	2.83	3.671(6)	145
C13–H132···Cl6^{vi}	0.96	2.60	3.203(6)	121
C14–H141···Cl6	0.96	2.53	3.419(6)	154
C21–H215···Cl5^{iii}	0.97	2.78	3.619(3)	145
C22–H223···Cl3	0.97	2.78	3.500(3)	131
C22–H224···Cl4^{iii}	0.97	2.81	3.542(3)	133
C23–H232···Cl4^{iii}	0.96	2.82	3.488(3)	127
C24–H242···Cl3^{vi}	0.96	2.63	3.573(3)	166
C24–H243···Cl3	0.96	2.77	3.596(3)	144

Symmetry codes: (i) $-x, -y, -z + 1$; (ii) $x, -y, z - 1/2$; (iii) $x, y + 1, z$; (iv) $x, -y + 1, z + 1/2$; (v) $-x + 1/2, y + 1/2, -z + 3/2$; (vi) $x, -y + 1, z - 1/2$; (vii) $-x, y, -z + 1/2$.

Table S6 Hydrogen bonds geometries (Å, °) for **2** at 295 K.

	D–H	H···A	D···A	D–H···A
N1–H13···Cl1^{i}	0.89	2.82	3.455(4)	129
N1–H13···Cl2^{ii}	0.89	2.59	3.322(4)	140
N1–H12···Cl4^{i}	0.89	2.36	3.186(4)	154
N1–H11···Cl5^{iii}	0.89	2.40	3.243(4)	159
N2–H21···Cl4^{ii}	0.98	2.49	3.299(4)	139
N2–H21···Cl5	0.98	2.90	3.557(4)	125
C1–H14···Cl3^{iv}	0.97	2.72	3.428(6)	130
C1–H15···Cl4^{ii}	0.97	2.83	3.600(5)	137
C4–H41···Cl3^{ii}	0.96	2.78	3.688(6)	158

Symmetry codes: (i) $-x + 3/2, -y + 1, z + 1/2$; (ii) $-x + 1/2, -y + 1, z + 1/2$; (iii) $-x + 1, y + 1/2, -z + 1/2$; (iv) $x + 1, y, z$.

Table S7 Hydrogen bonds geometries (Å, °) for **3** at 295 K.

	D–H	H···A	D···A	D–H···A
N11–H111···Cl2	0.86	2.63	3.304(3)	136
N11–H112···Cl6	0.86	2.44	3.242(3)	155
N21–H212···Cl2	0.86	2.83	3.522(4)	138
N21–H211···Cl6	0.86	2.84	3.376(4)	122
N21–H211···Cl9	0.86	2.79	3.443(3)	134
N31–H311···Cl5	0.86	2.74	3.416(3)	137
N31–H312···Cl7^{i}	0.86	2.70	3.411(3)	141
C23–H232···Cl5^{ii}	0.96	2.82	3.702(4)	153
C23–H233···Cl7^{iii}	0.96	2.71	3.582(4)	151
C12–H121···N13	0.96	2.51	2.854(5)	101
C14–H141···N12	0.96	2.59	2.911(5)	100
C22–H221···N23	0.96	2.57	2.905(5)	101
C24–H241···N22	0.96	2.48	2.845(5)	102
C32–H321···N33	0.96	2.52	2.875(5)	102
C34–H341···N32	0.96	2.55	2.886(5)	100

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

Table S8 Hydrogen bonds geometries (Å, °) for **4** at 295 K.

	D–H	H···A	D···A	D–H···A
N11–H112···Cl5^{i}	0.86	2.75	3.460(6)	140
C12–H121···N13	0.96	2.52	2.876(8)	102
C14–H141···N12	0.96	2.53	2.888(8)	102
C22–H221···N23	0.96	2.54	2.903(8)	103
C24–H241···N22	0.96	2.51	2.881(9)	103

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

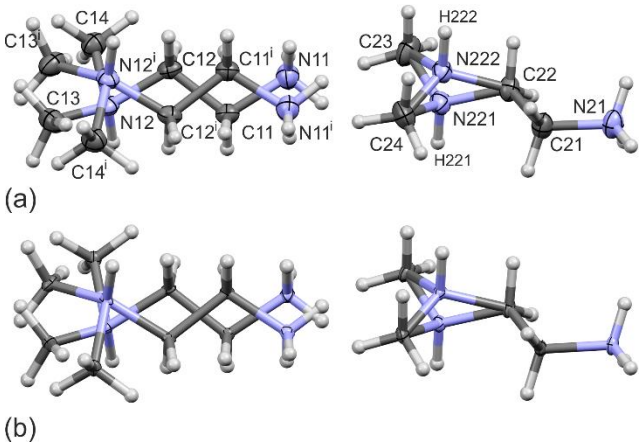

Figure S1 Disordered $[(CH_3)_2NH(CH_2)_2NH_3]^{2+}$ cations in **1** at 295 (a) and 100 K (b). The refined occupation factors for two sites of the split N22H22 group: 0.66 (N221 and H221) and 0.34 (N222 and H222) at 295 K, and 0.81 (N221 and H221) and 0.19 (N222 and H222) at 100 K. The same atom labelling scheme was used at both 295 and 100 K. Displacement ellipsoids are plotted at the 25% probability level. Symmetry code: (i) $-x$, y, $-z + 1/2$.

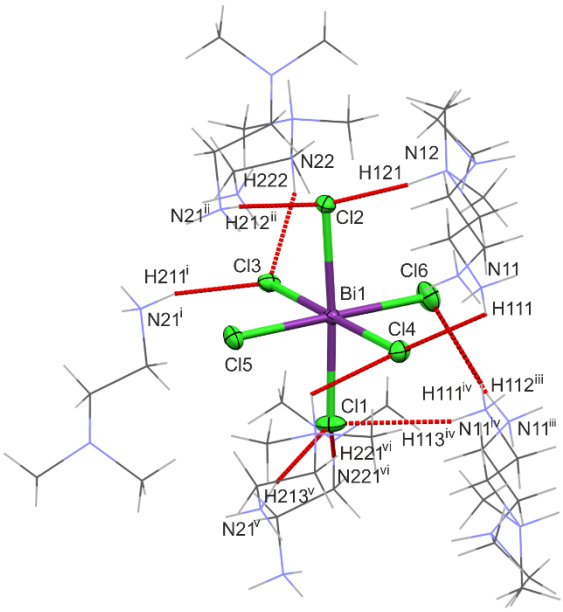

Figure S2 N–H···Cl hydrogen bonds, represented by the dashed red lines, in **1** at 295 K (see Table S5). Displacement ellipsoids are plotted at the 25% probability level. Symmetry codes: (i) –*x* + 1/2, *y* – 1/2, –*z* + 3/2; (ii) *x*, –*y* + 1, *z* – 1/2; (iii) *x*, –*y*, *z* + 1/2; (iv) –*x*, –*y*, –*z* + 1; (v) *x*, *y* – 1, *z*; (vi) *x*, –*y* + 1, *z* + 1/2.

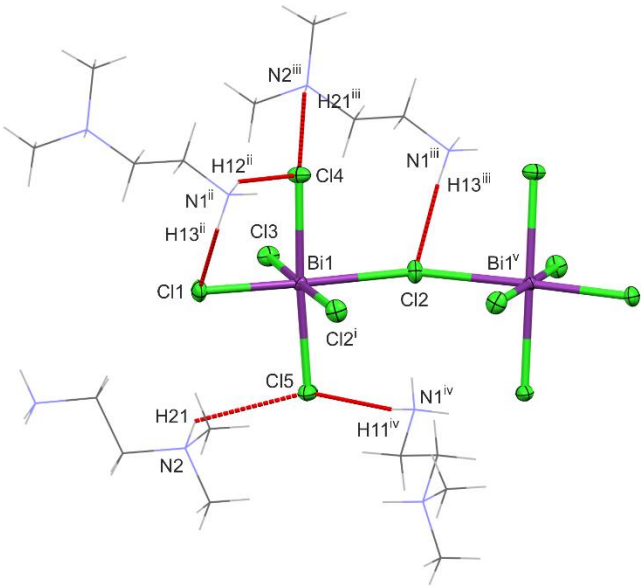

Figure S3 N–H···Cl hydrogen bonds, represented by the dashed red lines, in **2** at 295 K (see Table S6). Displacement ellipsoids are plotted at the 25% probability level. Symmetry codes: (i) *x* + 1/2, –*y* + 1/2, –*z*; (ii) –*x* + 3/2, –*y* + 1, *z* – 1/2; (iii) –*x* + 1/2, –*y* + 1, *z* – 1/2; (iv) –*x* + 1, *y* – 1/2, –*z* + 1/2; (v) *x* – 1/2, –*y* + 1/2, –*z*.

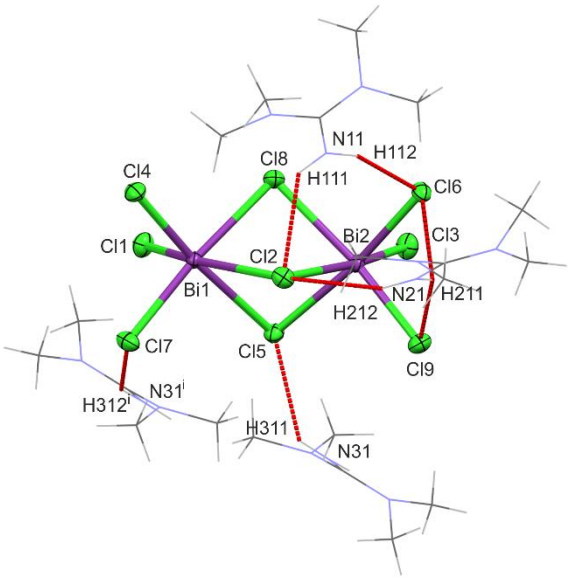

Figure S4 N–H···Cl hydrogen bonds, represented by the dashed red lines, in **3** at 295 K (see Table S7). Displacement ellipsoids are plotted at the 25% probability level. Symmetry code: (i) *–x*, *–y* + 1, *–z* + 1.

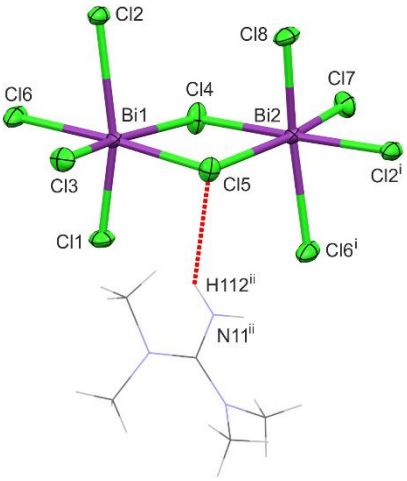

Figure S5 N–H···Cl hydrogen bond, represented by the dashed red line, in **4** at 295 K (see Table S8). Displacement ellipsoids are plotted at the 25% probability level. Symmetry codes: (i) *x* + 1, *y*, *z*; (ii) *–x* + 1, *–y* + 1, *–z* + 1.

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