Table S1. Crystal data and structure refinement for NH2CH32ZnBr4_150K_a.

Identification code	NH2CH32ZnBr4_150K_a	
Empirical formula	C4 H16 Br4 N2 Zn	
Formula weight	477.20	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 8.6262(3) Å	α= 90°.
	b = 11.9760(4) Å	β= 90.3690(10)°.
	c = 13.6877(5) Å	γ = 90°.
Volume	1414.01(9) $Å^3$	
Z	4	
Density (calculated)	2.242 Mg/m^3	
Absorption coefficient	13.000 mm^{-1}	
F(000)	896	
Crystal size	0.237 x 0.204 x 0.106 mm^3	
Theta range for data collection	2.260 to 28.281°.	
Index ranges	-11<=h<=11, -15<=k<=15, -18<=l<=18	
Reflections collected	26223	
Independent reflections	3503 [R(int) = 0.0559]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.4159	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3503 / 0 / 104	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0214, wR2 = 0.0455	
R indices (all data)	R1 = 0.0268, wR2 = 0.0471	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.559 and -0.392 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for NH2CH32ZnBr4_150K_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zn(1)	3261(1)	7035(1)	4226(1)	21(1)
Br(1)	3142(1)	5038(1)	4062(1)	26(1)
Br(2)	3070(1)	7586(1)	5915(1)	28(1)
Br(3)	5798(1)	7700(1)	3701(1)	28(1)
Br(4)	1253(1)	7886(1)	3281(1)	33(1)
N(1)	2874(2)	4927(2)	6606(2)	29(1)
N(2)	2054(2)	6892(2)	1035(2)	32(1)
C(1)	3443(3)	5019(2)	7623(2)	32(1)
C(2)	1745(4)	5695(3)	1155(2)	49(1)
C(3)	1171(3)	4792(3)	6534(2)	46(1)
C(4)	3725(3)	7173(3)	932(3)	46(1)

Table S3. Bond lengths [Å] and angles [°] for NH2CH32ZnBr4_150K_a.

Zn(1)-Br(4)	2.3837(4)
Zn(1)-Br(1)	2.4052(4)
Zn(1)-Br(2)	2.4117(4)
Zn(1)-Br(3)	2.4406(4)
N(1)-C(1)	1.477(3)
N(1)-C(3)	1.480(3)
N(1)-H(1NA)	0.9100
N(1)-H(1NB)	0.9100
N(2)-C(2)	1.468(4)
N(2)-C(4)	1.487(4)
N(2)-H(2NA)	0.9100
N(2)-H(2NB)	0.9100
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
Br(4)-Zn(1)-Br(1)	110.124(14)
Br(4)-Zn(1)-Br(2)	110.471(14)
Br(1)-Zn(1)-Br(2)	110.971(13)
Br(4)-Zn(1)-Br(3)	110.531(14)
Br(1)-Zn(1)-Br(3)	109.570(13)
Br(2)-Zn(1)-Br(3)	105.072(13)
C(1)-N(1)-C(3)	113.3(2)
C(1)-N(1)-H(1NA)	108.9
C(3)-N(1)-H(1NA)	108.9
C(1)-N(1)-H(1NB)	108.9
C(3)-N(1)-H(1NB)	108.9
H(1NA)-N(1)-H(1NB)	107.7
C(2)-N(2)-C(4)	114.1(2)
C(2)-N(2)-H(2NA)	108.7
C(4)-N(2)-H(2NA)	108.7
C(2)-N(2)-H(2NB)	108.7
C(4)-N(2)-H(2NB)	108.7
H(2NA)-N(2)-H(2NB)	107.6
N(1)-C(1)-H(1A)	109.5
N(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
N(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5

N(2)-C(2)-H(2A)	109.5
N(2)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
N(2)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
N(1)-C(3)-H(3A)	109.5
N(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
N(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
N(2)-C(4)-H(4A)	109.5
N(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
N(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for NH2CH32ZnBr4_150K_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	22(1)	21(1)	21(1)	0(1)	-1(1)	-1(1)
Br(1)	26(1)	21(1)	29(1)	-3(1)	0(1)	-1(1)
Br(2)	31(1)	30(1)	24(1)	-7(1)	3(1)	1(1)
Br(3)	27(1)	30(1)	28(1)	1(1)	5(1)	-7(1)
Br(4)	34(1)	31(1)	35(1)	5(1)	-11(1)	6(1)
N(1)	24(1)	35(1)	28(1)	2(1)	5(1)	0(1)
N(2)	28(1)	36(1)	32(1)	2(1)	-6(1)	9(1)
C(1)	32(1)	36(2)	29(1)	-2(1)	3(1)	1(1)
C(2)	52(2)	39(2)	55(2)	8(2)	-4(2)	2(1)
C(3)	22(1)	67(2)	50(2)	1(2)	-1(1)	-9(1)
C(4)	33(2)	47(2)	60(2)	2(2)	-3(2)	8(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for NH2CH32ZnBr4_150K_a.

	x	y	z	U(eq)
H(1NA)	3338	4332	6317	35
H(1NB)	3155	5552	6272	35
H(2NA)	1672	7264	1561	39
H(2NB)	1536	7140	496	39
H(1A)	4570	5121	7623	48
H(1B)	3184	4336	7981	48
H(1C)	2952	5661	7940	48
H(2A)	626	5575	1220	73
H(2B)	2277	5422	1744	73
H(2C)	2125	5289	584	73
H(3A)	858	4781	5844	69
H(3B)	661	5416	6865	69
H(3C)	867	4088	6844	69
H(4A)	4147	6785	362	70
H(4B)	4289	6938	1521	70
H(4C)	3839	7981	845	70

Table S6. Crystal data and structure refinement for 2_300K_a.

Identification code	2_300K_a	
Empirical formula	C4 H16 Br4 N2 Zn	
Formula weight	477.20	
Temperature	300(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 8.7517(13) Å	α= 90°.
	b = 12.0041(15) Å	β= 90°.
	c = 13.911(2) Å	γ = 90°.
Volume	1461.5(4) $Å^3$	
Z	4	
Density (calculated)	2.169 Mg/m^3	
Absorption coefficient	12.578 mm^{-1}	
F(000)	896	
Crystal size	0.187 x 0.166 x 0.065 mm^3	
Theta range for data collection	2.241 to 28.473°.	
Index ranges	-11<=h<=11, -15<=k<=16, -18<=l<=18	
Reflections collected	31817	
Independent reflections	3663 [R(int) = 0.0598]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.3235	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3663 / 0 / 105	
Goodness-of-fit on F^2	0.965	
Final R indices [I>2sigma(I)]	R1 = 0.0326, wR2 = 0.0832	
R indices (all data)	R1 = 0.0476, wR2 = 0.0916	
Extinction coefficient	0.0134(5)	
Largest diff. peak and hole	0.823 and -0.929 $e.Å^{-3}$	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2_300K_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	6964(1)	2384(1)	5878(1)	60(1)
Br(2)	8740(1)	2127(1)	3268(1)	72(1)
Br(3)	6839(1)	4948(1)	4062(1)	57(1)
Br(4)	4236(1)	2287(1)	3708(1)	60(1)
Zn(1)	6744(1)	2951(1)	4216(1)	45(1)
N(1)	2864(4)	4940(3)	3400(3)	60(1)
N(2)	2961(4)	1856(3)	6031(3)	70(1)
C(1)	1193(6)	4771(6)	3492(5)	100(2)
C(2)	3415(6)	5032(4)	2407(3)	69(1)
C(3)	3277(7)	669(5)	6137(5)	104(2)
C(4)	1334(7)	2154(5)	5928(5)	95(2)

Table S8. Bond lengths [Å] and angles [°] for 2_300K_a.

Br(1)-Zn(1)	2.4186(7)
Br(2)-Zn(1)	2.4018(7)
Br(3)-Zn(1)	2.4075(6)
Br(4)-Zn(1)	2.4401(6)
N(1)-C(2)	1.467(6)
N(1)-C(1)	1.482(6)
N(1)-H(1NA)	0.8900
N(1)-H(1NB)	0.8900
N(2)-C(3)	1.459(7)
N(2)-C(4)	1.475(7)
N(2)-H(2NA)	0.8900
N(2)-H(2NB)	0.8900
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600
C(4)-H(4C)	0.9600
Br(2)-Zn(1)-Br(3)	109.64(2)
Br(2)-Zn(1)-Br(1)	110.59(3)
Br(3)-Zn(1)-Br(1)	111.26(2)
Br(2)-Zn(1)-Br(4)	111.11(3)
Br(3)-Zn(1)-Br(4)	109.31(2)
Br(1)-Zn(1)-Br(4)	104.84(2)
C(2)-N(1)-C(1)	114.6(4)
C(2)-N(1)-H(1NA)	108.6
C(1)-N(1)-H(1NA)	108.6
C(2)-N(1)-H(1NB)	108.6
C(1)-N(1)-H(1NB)	108.6
H(1NA)-N(1)-H(1NB)	107.6
C(3)-N(2)-C(4)	115.4(4)
C(3)-N(2)-H(2NA)	108.4
C(4)-N(2)-H(2NA)	108.4
C(3)-N(2)-H(2NB)	108.4
C(4)-N(2)-H(2NB)	108.4
H(2NA)-N(2)-H(2NB)	107.5
N(1)-C(1)-H(1A)	109.5
N(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
N(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5

N(1)-C(2)-H(2A)	109.5
N(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
N(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
N(2)-C(3)-H(3A)	109.5
N(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
N(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
N(2)-C(4)-H(4A)	109.5
N(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
N(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 2_300K_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	70(1)	62(1)	48(1)	12(1)	-10(1)	1(1)
Br(2)	73(1)	68(1)	76(1)	-11(1)	24(1)	11(1)
Br(3)	61(1)	45(1)	64(1)	7(1)	-3(1)	-3(1)
Br(4)	57(1)	61(1)	62(1)	-1(1)	-14(1)	-13(1)
Zn(1)	47(1)	45(1)	42(1)	-1(1)	0(1)	-1(1)
N(1)	55(2)	68(2)	58(2)	-7(2)	-11(2)	1(2)
N(2)	63(2)	76(3)	71(3)	7(2)	13(2)	-16(2)
C(1)	59(3)	141(6)	100(5)	-4(4)	3(3)	-17(3)
C(2)	72(3)	75(3)	61(3)	5(2)	-10(2)	-1(2)
C(3)	117(5)	73(4)	120(5)	21(4)	4(4)	-6(3)
C(4)	62(3)	103(4)	121(5)	2(4)	7(3)	-6(3)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2_300K_a.

	x	y	z	U(eq)
H(1NA)	3120	5557	3715	72
H(1NB)	3340	4372	3682	72
H(2NA)	3462	2106	5518	84
H(2NB)	3333	2210	6543	84
H(1A)	665	5388	3205	150
H(1B)	925	4720	4159	150
H(1C)	906	4095	3170	150
H(2A)	3226	4345	2074	104
H(2B)	4492	5183	2409	104
H(2C)	2887	5628	2088	104
H(3A)	2699	378	6666	155
H(3B)	4347	562	6256	155
H(3C)	2993	287	5557	155
H(4A)	1247	2931	5777	143
H(4B)	808	2003	6519	143
H(4C)	888	1721	5420	143