Supporting Information

Efficient Broad-band Emission from Contorted Purely Corner-Shared One Dimensional (1D) Organic Lead Halide Perovskite

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Materials:

Lead (II) bromide (99%), Lead (II) chloride (99%), Hydrochloric acid (37%) were purchased from Sigma Aldrich. Dimethyl sulfoxide (DMSO), Dichloromethane (DCM, anhydrous), 1-(2-Aminoethyl) piperazine and Hydrobromic acid (47%) were purchased from TCI Chemicals. All chemicals were used as purchased without further purification.

Synthesis of powdered PzPbBr 1D Perovskites:

For the preparation of powdered $(Pz)_2PbBr_{10}$ perovskite, 1 mmol (365 mg) of $PbBr_2$ was dissolved in 3 mL of hydrobromic acid. To this, 1 mmol (140 µL) 1-(2-Aminoethyl) piperazine was added drop by drop. The solution turns turbid white immediately after addition and

precipitates into white perovskite powder gradually. The resulting precipitate was washed with diethyl ether three times and dried under vacuum at 60°C for further recrystallization.

Synthesis of Single Crystals of PzPbBr 1D Perovskites:

For the synthesis of single crystals of $(Pz)_2Pb_2Br_{10}$ perovskite, 2 mmol (730 mg) of $PbBr_2$ was dissolved in 10 mL of hydrobromic acid. To this transparent solution, 2 mmol (280 µL) 1-(2-Aminoethyl) piperazine was added in a dropwise manner. When the solution becomes turbid white, it was heated at 170 °C in an oil bath for 30 minutes under observation till the solution was clear. It was then allowed to cool naturally while still in oil bath. The natural drop in temperature leads to the formation of colourless bar-shaped crystal visible in the mother liquor. The crystals were filtered using a vacuum pump and washed repeatedly with dichloromethane for further characterization.

Synthesis of Single Crystals of PzPbCl 1D Perovskites:

Powdered $(Pz)_2Pb_2Cl_{10}$ perovskite was prepared by dissolving 1 mmol (278 mg) of $PbCl_2$ in 5 mL of hydrochloric acid (37%) followed by dropwise addition of 1 mmol (140 µL) 1-(2-Aminoethyl) piperazine. The obtained powder was filtered using a vacuum pump and washed 3 times with diethyl ether. For recrystallization of synthesised perovskite considerable amount was dissolved in dimethyl sulfoxide by heating at 150 °C. The solution was cooled naturally and kept in ambient atmosphere for several days to grow single crystals. The obtained single crystals were washed repeatedly with diethyl ether for further analysis.

Synthesis of Single Crystals of $PzPbBr_{1-x}Cl_x$ 1D Perovskites:

For synthesis of mixed halide perovskite single crystals, 0.5 mmol (183 mg) of $PbBr_2$ was dissolved in a mixture of hydrobromic acid and hydrochloric acid with varying ratio 3:1, 1:1 and 1:3 respectively keeping the total acid volume 20 mL, To that solution mixture, 0.5 mmol (70 µL) of 1-(2-Aminoethyl) piperazine was added in dropwise manner. After a few minutes the whole solution becomes white turbid which was then heated in a pre-heated oil bath at 210°C till transparent solution. Then the clear solution was cooled slowly inside oil bath which give rise to mixed halide perovskite crystals. The obtained crystals were filtered using a vacuum pump and washed repeatedly with dichloromethane for further characterization.

Methods:

UV-Vis Absorbance was performed in a Shimadzu UV-VIS-NIR3600Plus spectrometer. Steady State PL and lifetime was measured using an Edinburgh FS5 spectrophotometer. PXRD

patterns were recorded using a PANalytic X'Pert Pro using Copper Ka radiation ((λ=1.5406 A^0). TGA measurements were performed using a TAG system (Mettler-Toledo, Model TGA/SDTA851e) and samples were heated in the range of 25-800^{0}C at a heating rate of 5^{0}C/min under nitrogen atmosphere. Raman spectroscopy was performed using a Renishaw InVia Raman spectrometer with an excitation laser at 633nm. Absolute quantum yield measurements were carried out in a Horiba JOBIN YVON Fluoromax-4 spectrometer with a calibrated integrating sphere attachment. Low-temperature PL measurements were performed on a homebuilt PL set up consisting of an excitation monochromator (Jobin Yvon Triax 180), an emission monochromator (Jobin Yvon iHR 320) and photomultiplier tube (PMT) as the detector with xenon lamp (450 W).

Single crystals X-ray intensity data measurements of compounds **AB_280818 (PzPbBr)** and **AB_190918 (PzPbCl)** were carried out on a Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer equipped with Incoatech multilayer mirrors optics. The intensity measurements were carried out at 100(2) K temperature with Mo micro-focus sealed tube diffraction source (MoK_α= 0.71073 Å). The X-ray generator was operated at 50 kV and 1.4. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 36 frames. Data were collected with ω scan width of 0.5° at different settings of φ and 2θ with a frame time of 10 secs keeping the sample-to-detector distance fixed at 5.00 cm. The X-ray data collection was monitored by APEX3 program (Bruker, 2016).[1] All the data were corrected for Lorentzian, polarization and absorption effects using SAINT and SADABS programs (Bruker, 2016).[1] Using APEX3 (Bruker) program suite, the structure was solved with the ShelXS-97 (Sheldrick, 2008)[2] structure solution program, using direct methods. The model was refined with version of ShelXL-2013 (Sheldrick, 2015)[3] using Least Squares minimisation. All the hydrogen atoms were placed in a geometrically idealized position and constrained to ride on its parent atoms. An *ORTEP* III[4] view of compounds was drawn with 50% probability displacement ellipsoids and H atoms are shown as small spheres of arbitrary radii.

References

1. Bruker (2016). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
2. Sheldrick, G. M. A short history of *SHELX***.** *Acta Crystallogr.*, **2008**, *A64*, 112.

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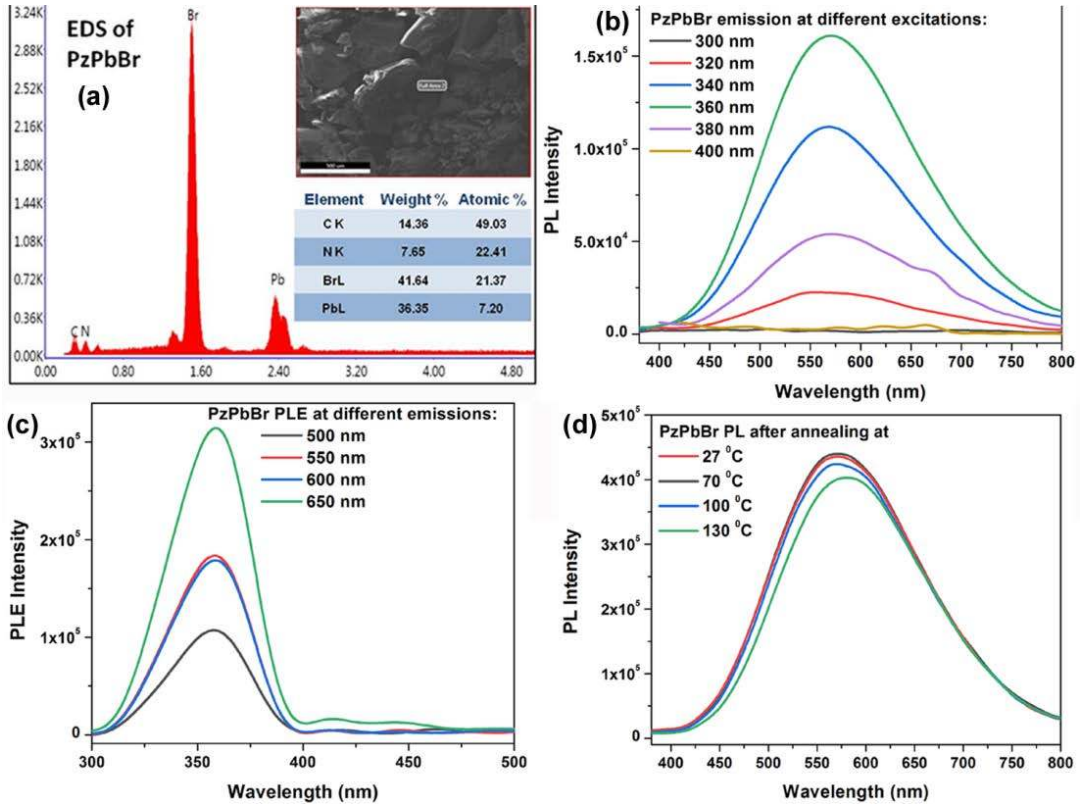


Figure S1: (a)EDS analysis of PzPbBr; (b) excitation dependent emission profile; (c) photoluminescence excitation (PLE) collected across broad emission band; (d) effect of thermal annealing on PL properties.

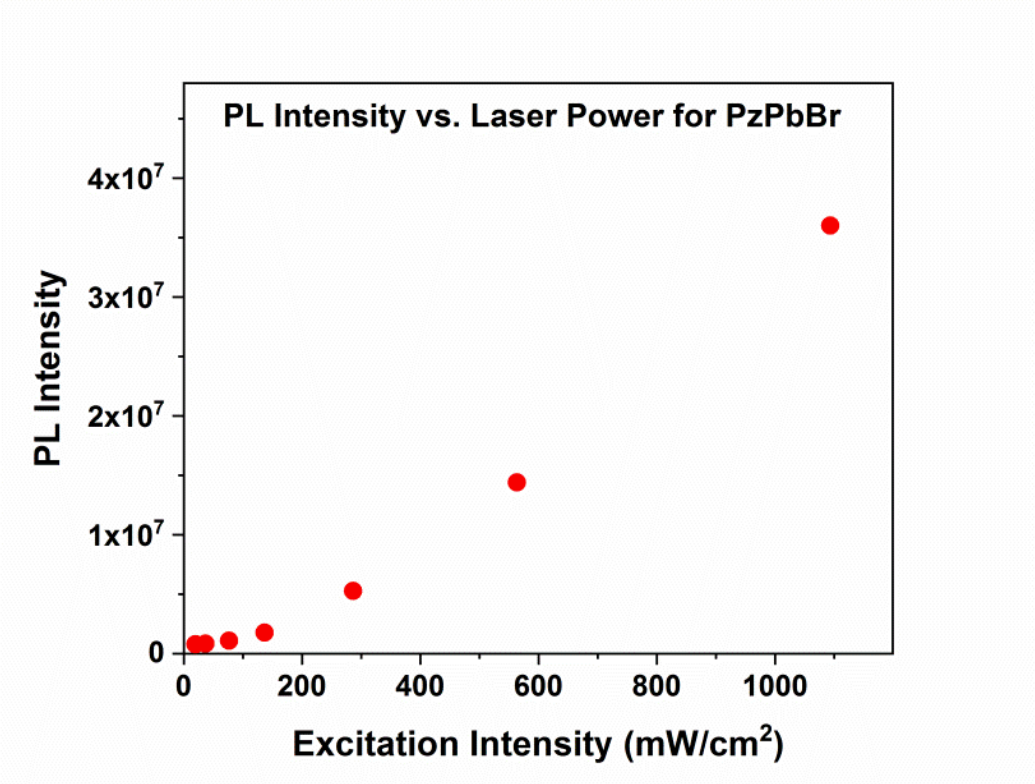
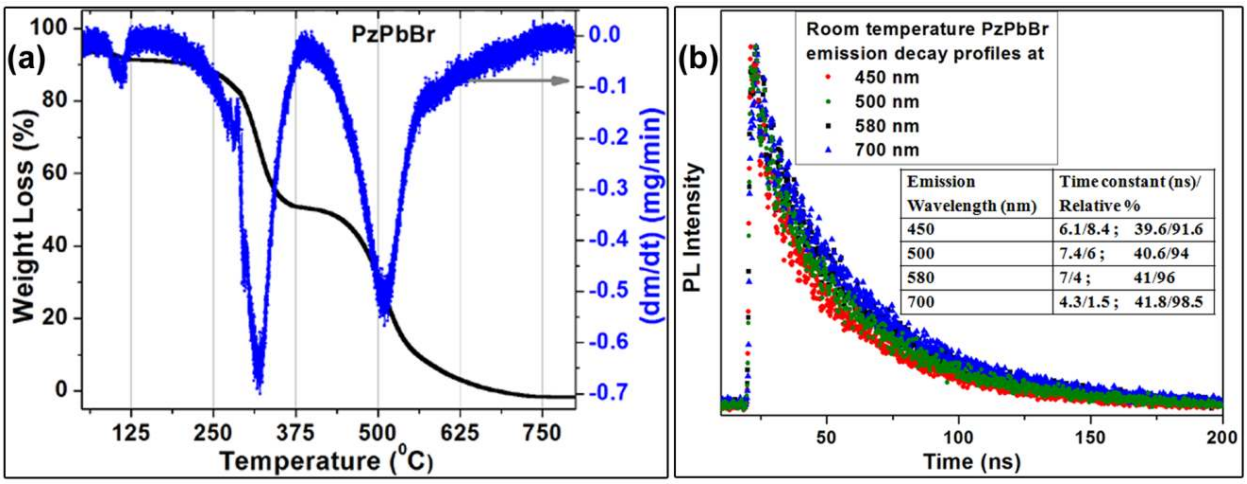


Figure S2: Intensity of broad emission increases as the excitation laser power is increased over three orders of magnitude with no signs of saturation, indicating the intrinsic nature of the emissive states in PzPbBr perovskite.



Emission Wavelength (nm)	Time constant (ns)/ Relative %
450	6.1/8.4 ; 39.6/91.6
500	7.4/6 ; 40.6/94
580	7/4 ; 41/96
700	4.3/1.5 ; 41.8/98.5

Figure S3: (a) Thermogravimetric weight loss analysis of PzPbBr; (b)Room temperature time resolved PL decay curves for PzPbBr single crystals measured across the broad emission band. Inset Table shows major and minor components of the decay time constants.

Table S1: Low temperature average lifetime for AePzBr

Temperature (K)	Lifetime (ns)				Average Lifetime (ns)
	τ_1	τ_2	A_1	A_2	
100	354.80	1164.00	2.12	97.88	1158.69
160	102.50	541.70	2.90	97.10	539.23
190	145.00	345.80	6.33	93.67	340.27
220	74.02	244.90	3.69	96.31	242.94
250	116.40	176.30	34.69	65.31	160.75
280	49.52	93.78	37.58	62.42	83.10
300	26.60	60.65	35.00	65.00	54.14

$$Average\ Lifetime = \frac{a_1(\tau_1^2) + a_2(\tau_2^2)}{(a_1\tau_1 + a_2\tau_2)}$$

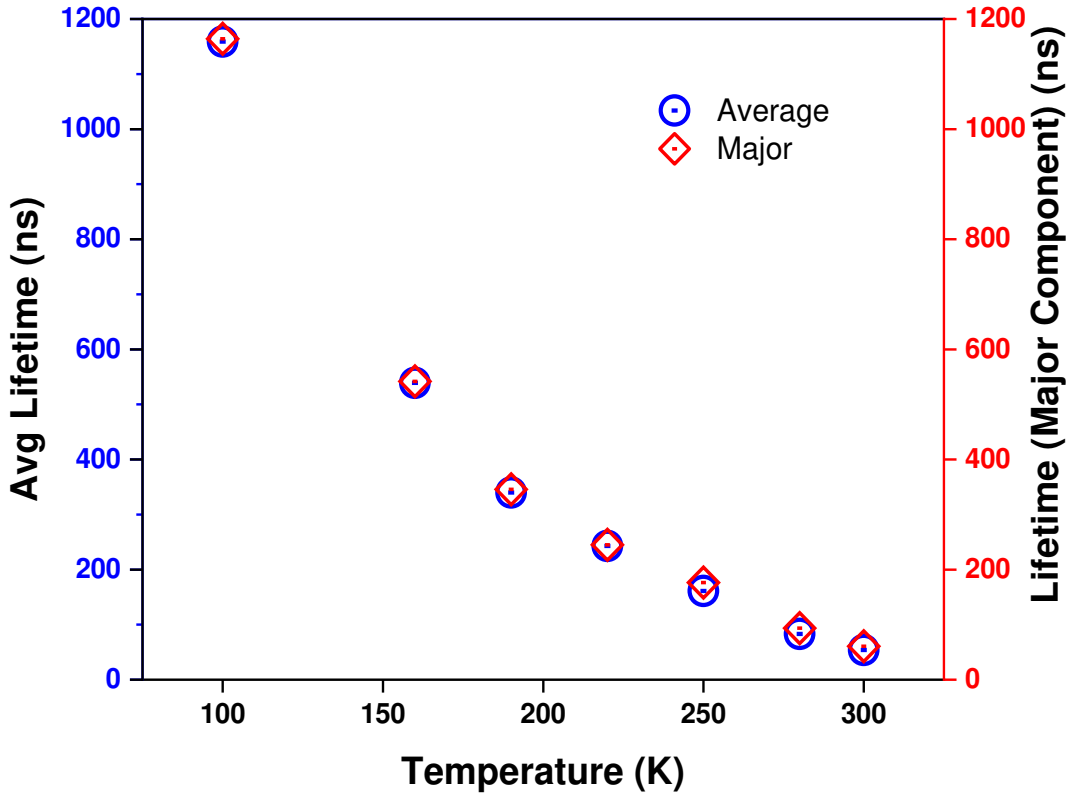


Figure S4: Temperature dependent PL lifetime with comparison of average and major component.

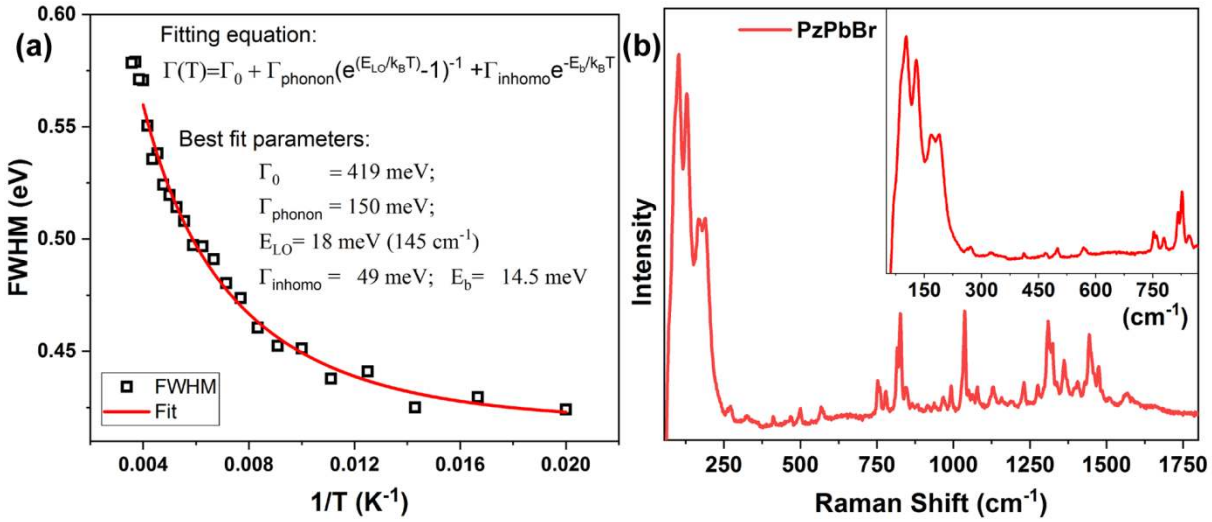


Figure S5: (a) Fitting of FWHM as a function of Temperature with its associated parameters and fitting equation; (b) Raman spectra of PzPbBr perovskite crystal excited with 633 nm laser.

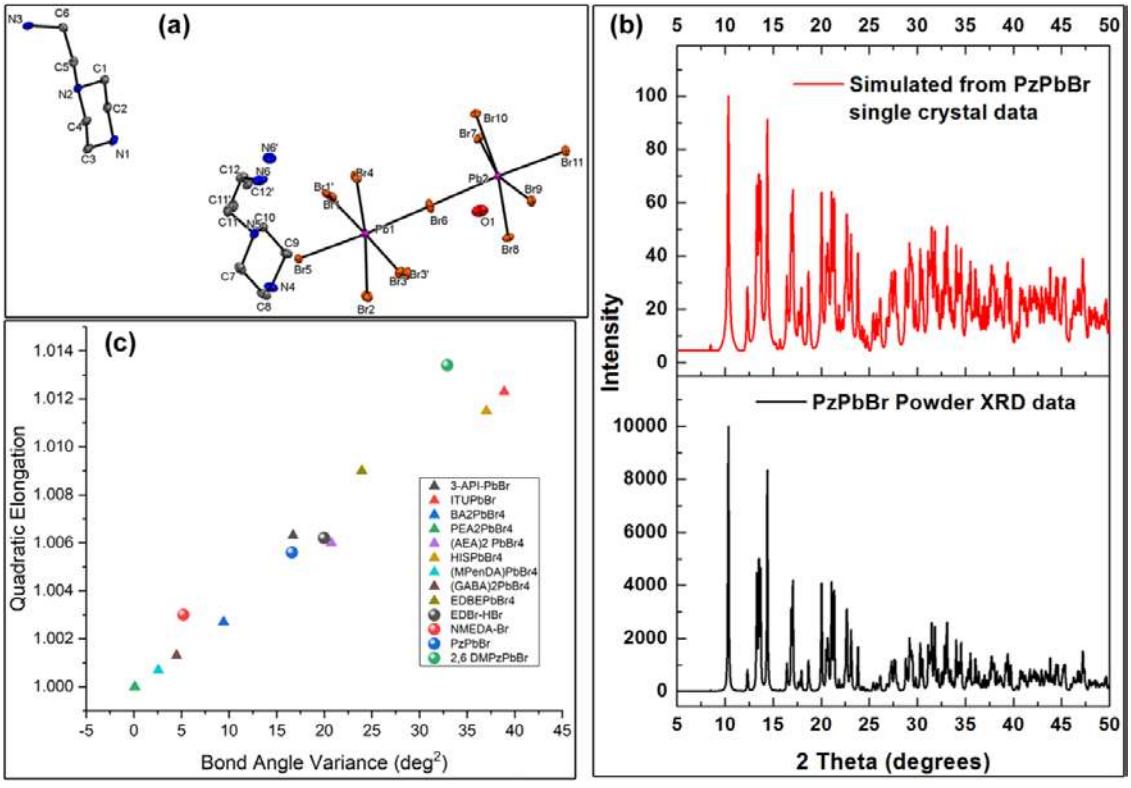


Figure S6: (a)Asymmetric unit of PzPbBr 1D chain perovskite; (b)comparison between powder XRD pattern of PzPbBr and XRD pattern simulated from single crystal data of PzPbBr; (c) structural distortion correlation for broad band emitting perovskites (2D: triangle; 1D: circles). References for compounds shown in panel c are provided below:

COMPOUND	REFERENCE
APIPbBr	1
ITUPbBr	2
BA_2PbBr_4	3
PEA_2PbBr_4	4
(AeA)2PbBr4	5
HISPbBr4	5
MpenDAPbBr4	5
GABA2PbBr4	5
EDBr-HBr	6
NMEDAPbBr	7
EDBEPbBr4	8
2,6DMPzPbBr	9

References

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Table S2: Comparison of bond angles and dihedral angles of PzPbBr with the reported 1D broad emitting perovskite with modest quantum yield.

1D perovskite Compounds	**Bond angles PbBrPb**	**Bond angles PbPbPb**	**Dihedral Angle**	**Quantum yield**
Ref (16) *Nat. Commun.* **2017**, *8*, 14051. Corner and Edge share	176.72 ˚	85 ˚	0 ˚	20%
Ref (8) *J. Am. Chem. Soc.* **2018**, *140*,13078.	165.84	180	0 ˚	12%
Ours PzPbBr	167.16 ˚ 180 ˚	90.87 ˚ 103.38 ˚	10.33 ˚ 12.04 ˚	9%

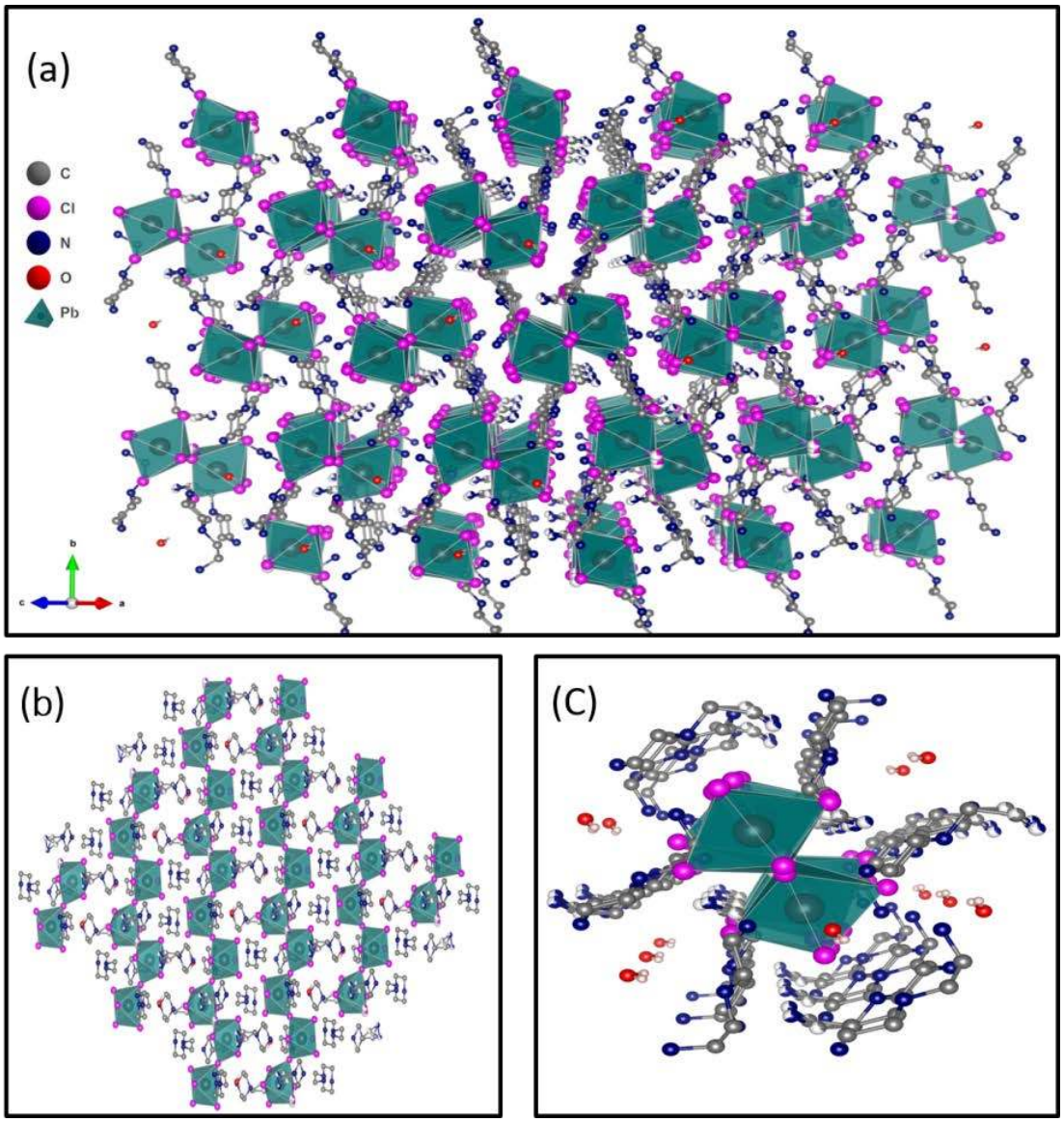

Figure S7: (a) Single crystal structure of PzPbCl; (b) top view; (c) sliced view highlighting the 1D contorted corner-shared structure with two octahedral unit wide chain surrounded by ligands and water molecule. H atoms have been omitted for clarity.

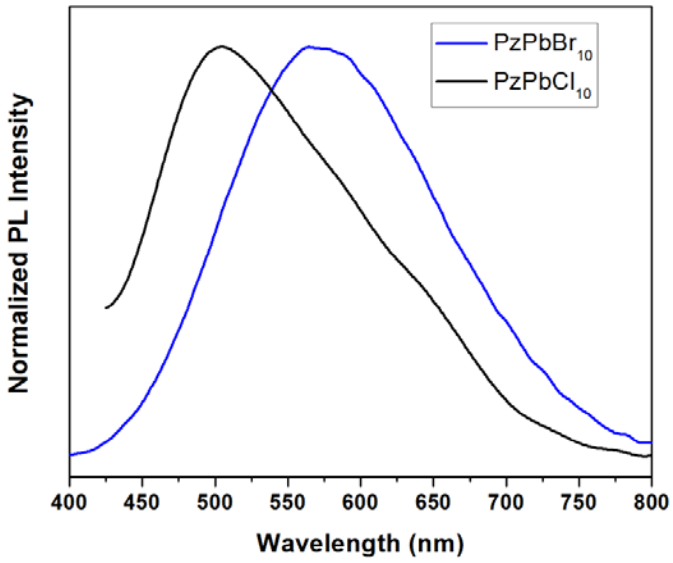

Figure S8: PL emission profile of PzPbBr and PzPbCl showing blue shifted emission for PzPbCl perovskite.

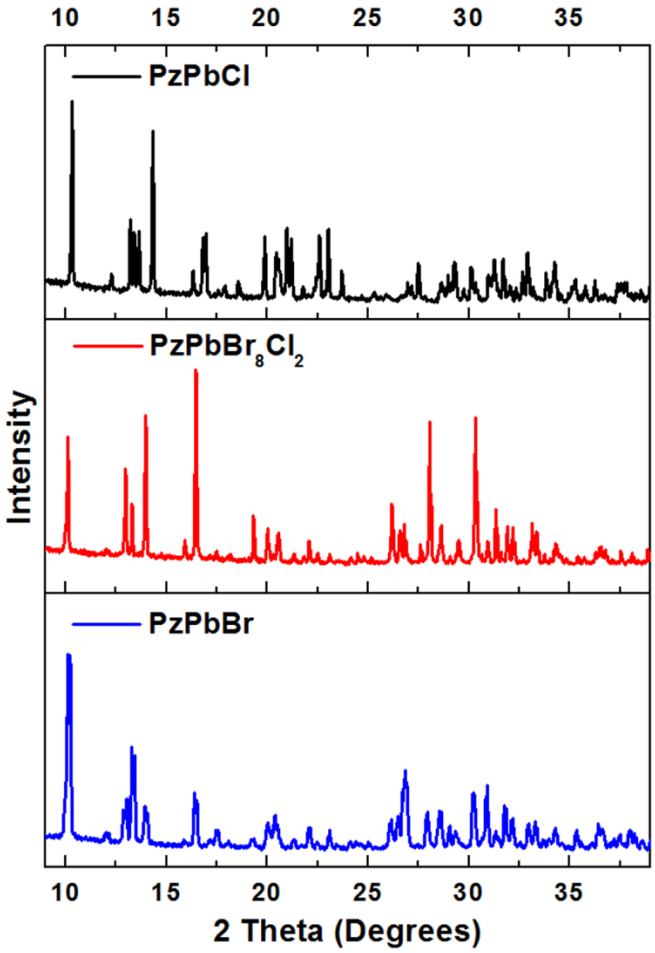

Figure S9: Comparison of PXRD pattern of $PzPbBr_{10}$, $PzPbCl_{10}$, and $PzPbBr_8Cl_2$ perovskite.

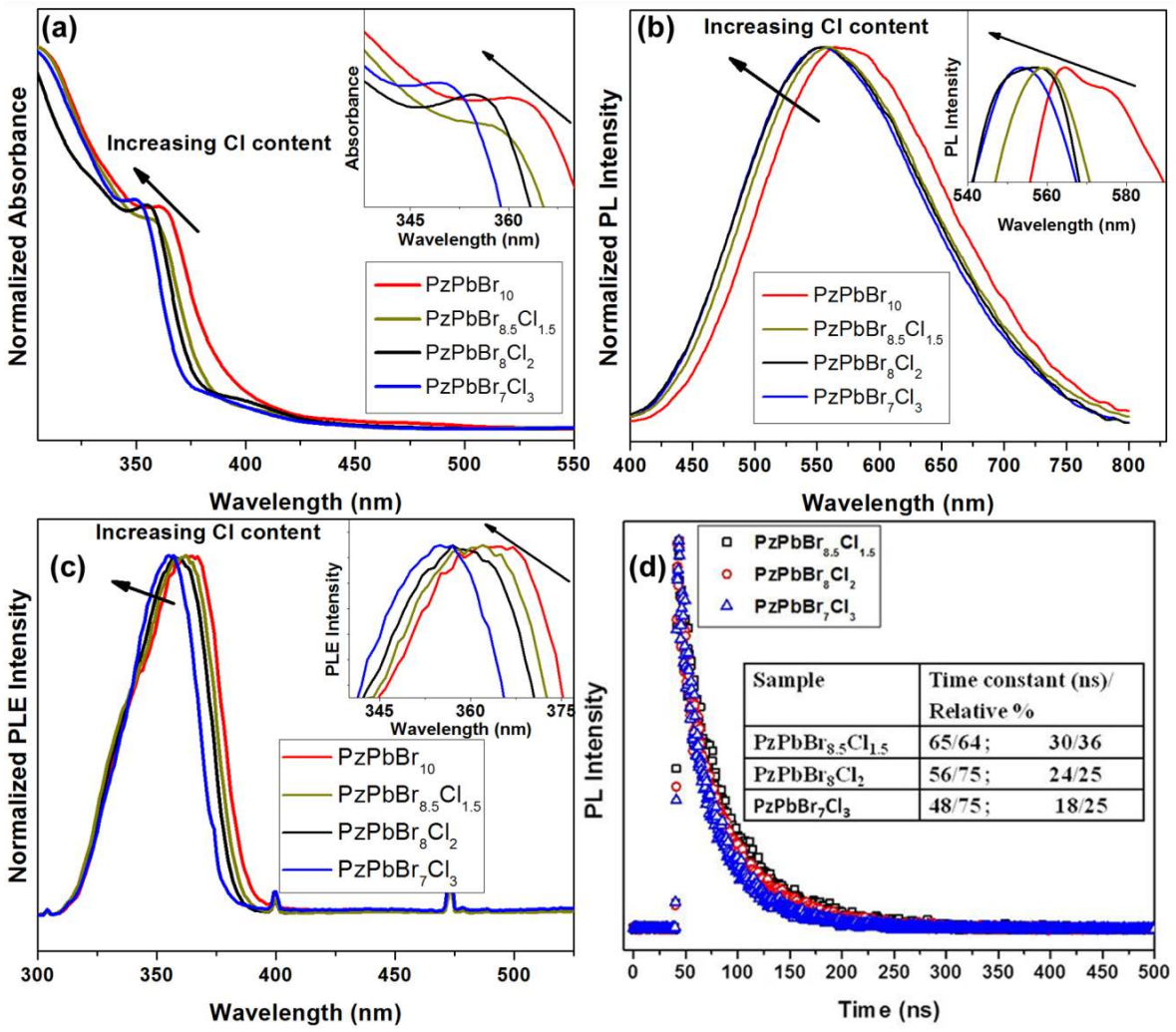

Figure S10: Comparison of (a) Absorbance; (b) PL emission; (c) PLE; (d) Lifetime analysis for PzPbBr and Br-Cl mixed halide perovskites showing blue shifted absorbance and emission with lifetime lengthening.

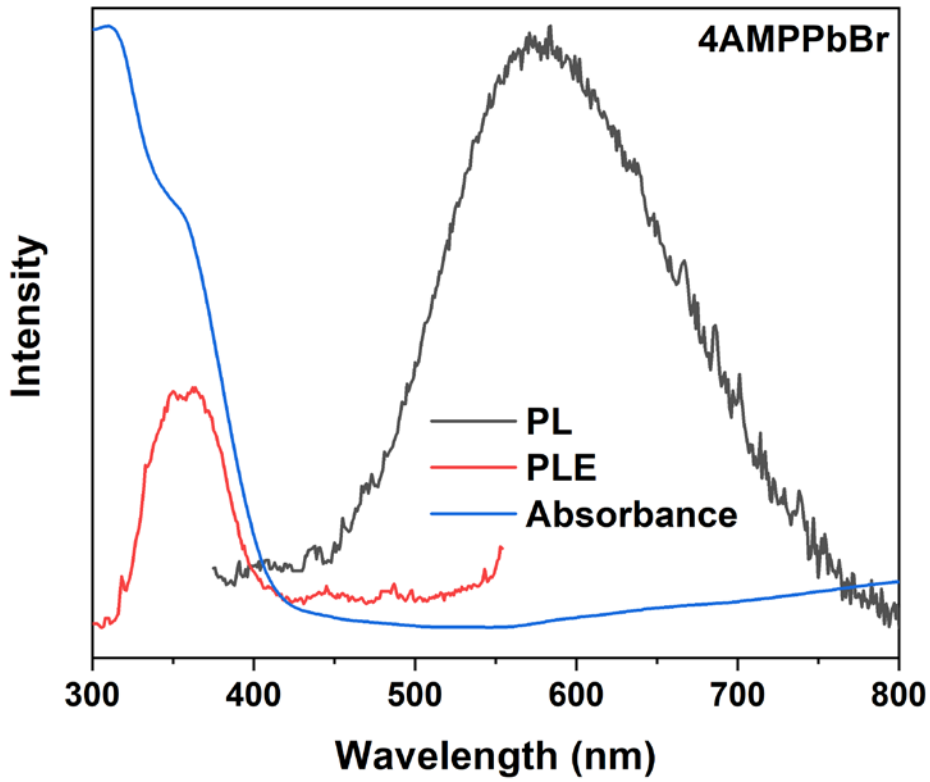

Figure S11: Optical characterization of purely edge shared broad band emitting 1D 4AMPPbBr perovskite.

Crystal structure Data:

1) Crystal data of **AB_280818 (PzPbBr):** $C_{12}H_{38}Br_{10}N_6OPb_2$ [Pb_2Br_{10}, 2($C_6H_{18}N_3$), H_2O], M = 1495.96, colorless block, 0.20 x 0.12 x 0.08 mm^3, monoclinic, space group $P2_1/c$, a = 13.7518(4) Å, b = 17.4924(6) Å, c = 13.7488(5) Å, β = 96.2380(10)°, V = 3287.72(19) $Å^3$, Z = 4, T = 100(2) K, $2\theta_{max}$= 56.592°, D_{calc} (g cm^{-3}) = 3.022, $F(000)$ = 2696, μ (mm^{-1}) = 22.400, 35698 reflections collected, 8112 unique reflections (R_{int} = 0.0314, R_{sig} = 0.0302), 7261 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.094, T_{max} = 0.267, 340 refined parameters, 70 restraints, Good of Fit = S = 1.079, $R1$ = 0.0207, $wR2$ = 0.0395 (all data R = 0.0268, $wR2$ = 0.0415), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.939, $\Delta\rho_{min}$= -1.081 (e $Å^{-3}$).

Table S3. Crystal data and structure refinement for mo_AB_280818_0m (PzPbBr)

Identification code	mo_AB_280818_0m	
Empirical formula	C12 H38 Br10 N6 O Pb2	
Formula weight	1495.96	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.7518(4) Å	□= 90°.
	b = 17.4924(6) Å	□= 96.2380(10)°.
	c = 13.7488(5) Å	□ = 90°.
Volume	3287.72(19) $Å^3$	
Z	4	
Density (calculated)	3.022 Mg/m^3	
Absorption coefficient	22.400 mm^{-1}	
F(000)	2696	
Crystal size	0.200 x 0.120 x 0.080 mm^3	
Theta range for data collection	2.506 to 28.296°.	
Index ranges	-17<=h<=18, -23<=k<=23, -17<=l<=18	
Reflections collected	35698	
Independent reflections	8112 [R(int) = 0.0314]	
Completeness to theta = 25.242°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.267 and 0.094	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8112 / 70 / 340	
Goodness-of-fit on F^2	1.079	
Final R indices [I>2sigma(I)]	R1 = 0.0207, wR2 = 0.0395	
R indices (all data)	R1 = 0.0268, wR2 = 0.0415	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.939 and -1.081 $e.Å^{-3}$	

Table S4. Bond lengths [Å] and angles [°] for mo_AB_280818_0m.

Pb(1)-Br(1')	2.894(3)
Pb(1)-Br(1)	2.909(3)
Pb(1)-Br(4)	2.9123(4)
Pb(1)-Br(5)	2.9336(4)
Pb(1)-Br(3)	2.99943(15)
Pb(1)-Br(3')	2.999(8)
Pb(1)-Br(3')#1	3.046(8)
Pb(1)-Br(6)	3.0991(4)
Pb(1)-Br(2)	3.1072(4)
Pb(2)-Br(11)	2.9358(4)
Pb(2)-Br(9)	2.9382(4)
Pb(2)-Br(8)	2.9387(4)
Pb(2)-Br(10)	2.9963(4)
Pb(2)-Br(6)	3.0456(4)
Pb(2)-Br(7)	3.17066(16)
Br(3)-Pb(1)#1	2.99947(15)
Br(3')-Br(3')#1	0.746(16)
Br(3')-Pb(1)#1	3.045(8)
Br(7)-Pb(2)#2	3.17071(17)
C(1)-N(2)	1.504(4)
C(1)-C(2)	1.516(5)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-N(1)	1.492(4)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
N(1)-C(3)	1.490(4)
N(1)-H(1C)	0.9100
N(1)-H(1D)	0.9100
C(3)-C(4)	1.507(5)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-N(2)	1.504(4)
C(4)-H(4C)	0.9900

C(4)-H(4D)	0.9900
N(2)-C(5)	1.515(4)
N(2)-H(2)	1.0000
C(5)-C(6)	1.512(5)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-N(3)	1.489(4)
C(6)-H(6D)	0.9900
C(6)-H(6E)	0.9900
N(3)-H(3C)	0.9100
N(3)-H(3D)	0.9100
N(3)-H(3E)	0.9100
C(7)-C(8)	1.503(6)
C(7)-N(5)	1.505(5)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-N(4)	1.488(5)
C(8)-H(8A)	1.06(4)
C(8)-H(8B)	0.86(5)
N(4)-C(9)	1.489(5)
N(4)-H(4A)	0.9100
N(4)-H(4B)	0.9100
C(9)-C(10)	1.508(5)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-N(5)	1.506(5)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
N(5)-C(11)	1.500(10)
N(5)-C(11')	1.519(14)
N(5)-H(5)	1.0000
C(11)-C(12)	1.502(11)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-N(6)	1.485(7)
C(12)-H(12A)	0.9900

C(12)-H(12B)	0.9900
N(6)-H(6A)	0.9100
N(6)-H(6B)	0.9100
N(6)-H(6C)	0.9100
C(11')-C(12')	1.521(15)
C(11')-H(11C)	0.9900
C(11')-H(11D)	0.9900
C(12')-N(6')	1.439(11)
C(12')-H(12C)	0.9900
C(12')-H(12D)	0.9900
N(6')-H(6'A)	0.9100
N(6')-H(6'B)	0.9100
N(6')-H(6'C)	0.9100
O(1)-H(1AW)	0.8856
O(1)-H(1BW)	0.8719

Br(1')-Pb(1)-Br(4)	89.45(5)
Br(1)-Pb(1)-Br(4)	82.73(5)
Br(1')-Pb(1)-Br(5)	85.48(6)
Br(1)-Pb(1)-Br(5)	81.26(6)
Br(4)-Pb(1)-Br(5)	90.156(11)
Br(1)-Pb(1)-Br(3)	172.55(3)
Br(4)-Pb(1)-Br(3)	91.288(9)
Br(5)-Pb(1)-Br(3)	94.366(7)
Br(1')-Pb(1)-Br(3')	172.52(16)
Br(4)-Pb(1)-Br(3')	95.55(16)
Br(5)-Pb(1)-Br(3')	100.03(16)
Br(1')-Pb(1)-Br(3')#1	173.26(16)
Br(4)-Pb(1)-Br(3')#1	87.08(15)
Br(5)-Pb(1)-Br(3')#1	88.76(16)
Br(3')-Pb(1)-Br(3')#1	14.2(3)
Br(1')-Pb(1)-Br(6)	84.46(6)
Br(1)-Pb(1)-Br(6)	89.24(6)
Br(4)-Pb(1)-Br(6)	94.089(11)
Br(5)-Pb(1)-Br(6)	169.037(11)
Br(3)-Pb(1)-Br(6)	95.636(8)

Br(3')-Pb(1)-Br(6)	89.62(16)
Br(3')#1-Pb(1)-Br(6)	101.53(16)
Br(1')-Pb(1)-Br(2)	88.54(5)
Br(1)-Pb(1)-Br(2)	94.80(5)
Br(4)-Pb(1)-Br(2)	173.980(11)
Br(5)-Pb(1)-Br(2)	84.031(10)
Br(3)-Pb(1)-Br(2)	90.715(8)
Br(3')-Pb(1)-Br(2)	87.02(16)
Br(3')#1-Pb(1)-Br(2)	94.34(15)
Br(6)-Pb(1)-Br(2)	91.362(11)
Br(11)-Pb(2)-Br(9)	81.560(10)
Br(11)-Pb(2)-Br(8)	93.396(11)
Br(9)-Pb(2)-Br(8)	95.127(10)
Br(11)-Pb(2)-Br(10)	94.656(10)
Br(9)-Pb(2)-Br(10)	92.038(10)
Br(8)-Pb(2)-Br(10)	169.925(11)
Br(11)-Pb(2)-Br(6)	176.689(11)
Br(9)-Pb(2)-Br(6)	96.145(11)
Br(8)-Pb(2)-Br(6)	84.410(11)
Br(10)-Pb(2)-Br(6)	87.793(11)
Br(11)-Pb(2)-Br(7)	84.439(7)
Br(9)-Pb(2)-Br(7)	165.603(8)
Br(8)-Pb(2)-Br(7)	89.014(8)
Br(10)-Pb(2)-Br(7)	85.753(7)
Br(6)-Pb(2)-Br(7)	97.982(8)
Pb(1)-Br(3)-Pb(1)#1	180.0
Br(3')#1-Br(3')-Pb(1)	86.4(12)
Br(3')#1-Br(3')-Pb(1)#1	79.4(12)
Pb(1)-Br(3')-Pb(1)#1	165.8(3)
Pb(2)-Br(6)-Pb(1)	167.170(14)
Pb(2)-Br(7)-Pb(2)#2	180.0
N(2)-C(1)-C(2)	110.6(3)
N(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1A)	109.5
N(2)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1B)	109.5

H(1A)-C(1)-H(1B)	108.1
N(1)-C(2)-C(1)	111.4(3)
N(1)-C(2)-H(2A)	109.3
C(1)-C(2)-H(2A)	109.3
N(1)-C(2)-H(2B)	109.3
C(1)-C(2)-H(2B)	109.3
H(2A)-C(2)-H(2B)	108.0
C(3)-N(1)-C(2)	111.5(3)
C(3)-N(1)-H(1C)	109.3
C(2)-N(1)-H(1C)	109.3
C(3)-N(1)-H(1D)	109.3
C(2)-N(1)-H(1D)	109.3
H(1C)-N(1)-H(1D)	108.0
N(1)-C(3)-C(4)	110.6(3)
N(1)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3A)	109.5
N(1)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	108.1
N(2)-C(4)-C(3)	110.5(3)
N(2)-C(4)-H(4C)	109.6
C(3)-C(4)-H(4C)	109.6
N(2)-C(4)-H(4D)	109.6
C(3)-C(4)-H(4D)	109.6
H(4C)-C(4)-H(4D)	108.1
C(1)-N(2)-C(4)	108.9(3)
C(1)-N(2)-C(5)	113.6(3)
C(4)-N(2)-C(5)	109.0(2)
C(1)-N(2)-H(2)	108.4
C(4)-N(2)-H(2)	108.4
C(5)-N(2)-H(2)	108.4
C(6)-C(5)-N(2)	115.9(3)
C(6)-C(5)-H(5A)	108.3
N(2)-C(5)-H(5A)	108.3
C(6)-C(5)-H(5B)	108.3
N(2)-C(5)-H(5B)	108.3

H(5A)-C(5)-H(5B)	107.4
N(3)-C(6)-C(5)	113.7(3)
N(3)-C(6)-H(6D)	108.8
C(5)-C(6)-H(6D)	108.8
N(3)-C(6)-H(6E)	108.8
C(5)-C(6)-H(6E)	108.8
H(6D)-C(6)-H(6E)	107.7
C(6)-N(3)-H(3C)	109.5
C(6)-N(3)-H(3D)	109.5
H(3C)-N(3)-H(3D)	109.5
C(6)-N(3)-H(3E)	109.5
H(3C)-N(3)-H(3E)	109.5
H(3D)-N(3)-H(3E)	109.5
C(8)-C(7)-N(5)	111.3(3)
C(8)-C(7)-H(7A)	109.4
N(5)-C(7)-H(7A)	109.4
C(8)-C(7)-H(7B)	109.4
N(5)-C(7)-H(7B)	109.4
H(7A)-C(7)-H(7B)	108.0
N(4)-C(8)-C(7)	110.0(3)
N(4)-C(8)-H(8A)	107(2)
C(7)-C(8)-H(8A)	110(2)
N(4)-C(8)-H(8B)	106(3)
C(7)-C(8)-H(8B)	111(3)
H(8A)-C(8)-H(8B)	112(4)
C(8)-N(4)-C(9)	109.9(3)
C(8)-N(4)-H(4A)	109.7
C(9)-N(4)-H(4A)	109.7
C(8)-N(4)-H(4B)	109.7
C(9)-N(4)-H(4B)	109.7
H(4A)-N(4)-H(4B)	108.2
N(4)-C(9)-C(10)	110.0(3)
N(4)-C(9)-H(9A)	109.7
C(10)-C(9)-H(9A)	109.7
N(4)-C(9)-H(9B)	109.7
C(10)-C(9)-H(9B)	109.7

H(9A)-C(9)-H(9B)	108.2
N(5)-C(10)-C(9)	110.7(3)
N(5)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10A)	109.5
N(5)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	108.1
C(11)-N(5)-C(7)	105.5(5)
C(11)-N(5)-C(10)	113.2(6)
C(7)-N(5)-C(10)	110.0(3)
C(7)-N(5)-C(11')	116.1(7)
C(10)-N(5)-C(11')	110.4(8)
C(11)-N(5)-H(5)	109.3
C(7)-N(5)-H(5)	109.3
C(10)-N(5)-H(5)	109.3
N(5)-C(11)-C(12)	112.2(7)
N(5)-C(11)-H(11A)	109.2
C(12)-C(11)-H(11A)	109.2
N(5)-C(11)-H(11B)	109.2
C(12)-C(11)-H(11B)	109.2
H(11A)-C(11)-H(11B)	107.9
N(6)-C(12)-C(11)	110.5(7)
N(6)-C(12)-H(12A)	109.6
C(11)-C(12)-H(12A)	109.6
N(6)-C(12)-H(12B)	109.6
C(11)-C(12)-H(12B)	109.6
H(12A)-C(12)-H(12B)	108.1
C(12)-N(6)-H(6A)	109.5
C(12)-N(6)-H(6B)	109.5
H(6A)-N(6)-H(6B)	109.5
C(12)-N(6)-H(6C)	109.5
H(6A)-N(6)-H(6C)	109.5
H(6B)-N(6)-H(6C)	109.5
N(5)-C(11')-C(12')	118.3(11)
N(5)-C(11')-H(11C)	107.7
C(12')-C(11')-H(11C)	107.7

N(5)-C(11')-H(11D)	107.7
C(12')-C(11')-H(11D)	107.7
H(11C)-C(11')-H(11D)	107.1
N(6')-C(12')-C(11')	114.4(10)
N(6')-C(12')-H(12C)	108.7
C(11')-C(12')-H(12C)	108.7
N(6')-C(12')-H(12D)	108.7
C(11')-C(12')-H(12D)	108.7
H(12C)-C(12')-H(12D)	107.6
C(12')-N(6')-H(6'A)	109.5
C(12')-N(6')-H(6'B)	109.5
H(6'A)-N(6')-H(6'B)	109.5
C(12')-N(6')-H(6'C)	109.5
H(6'A)-N(6')-H(6'C)	109.5
H(6'B)-N(6')-H(6'C)	109.5
H(1AW)-O(1)-H(1BW)	107.9

Symmetry transformations used to generate equivalent atoms:

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

Table S5. Torsion angles [°] for mo_AB_280818_0m.

N(2)-C(1)-C(2)-N(1)	-56.0(4)
C(1)-C(2)-N(1)-C(3)	54.3(4)
C(2)-N(1)-C(3)-C(4)	-55.5(4)
N(1)-C(3)-C(4)-N(2)	58.7(4)
C(2)-C(1)-N(2)-C(4)	58.3(3)
C(2)-C(1)-N(2)-C(5)	-179.9(3)
C(3)-C(4)-N(2)-C(1)	-59.9(4)
C(3)-C(4)-N(2)-C(5)	175.6(3)
C(1)-N(2)-C(5)-C(6)	61.1(4)
C(4)-N(2)-C(5)-C(6)	-177.2(3)
N(2)-C(5)-C(6)-N(3)	71.1(4)
N(5)-C(7)-C(8)-N(4)	-57.7(4)
C(7)-C(8)-N(4)-C(9)	59.7(4)
C(8)-N(4)-C(9)-C(10)	-60.2(4)
N(4)-C(9)-C(10)-N(5)	58.3(4)
C(8)-C(7)-N(5)-C(11)	177.9(6)
C(8)-C(7)-N(5)-C(10)	55.4(4)
C(8)-C(7)-N(5)-C(11')	-178.3(8)
C(9)-C(10)-N(5)-C(11)	-173.3(5)
C(9)-C(10)-N(5)-C(7)	-55.5(4)
C(9)-C(10)-N(5)-C(11')	175.1(7)
C(7)-N(5)-C(11)-C(12)	158.5(7)
C(10)-N(5)-C(11)-C(12)	-81.1(9)
N(5)-C(11)-C(12)-N(6)	-76.6(10)
C(7)-N(5)-C(11')-C(12')	117.7(12)
C(10)-N(5)-C(11')-C(12')	-116.2(13)
N(5)-C(11')-C(12')-N(6')	82.4(16)

Symmetry transformations used to generate equivalent atoms:

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

2) Crystal data of **AB_190918 (PzPbCl):** $C_{12}H_{38}Cl_{10}N_6OPb_2$ [Pb_2Cl_{10}, 2($C_6H_{18}N_3$), H_2O], M = 1051.36, colorless block, 0.33 x 0.27 x 0.18 mm^3, monoclinic, space group $P2_1/c$, a = 13.3763(7) Å, b = 17.0747(8) Å, c = 13.1719(7) Å, β = 96.283(2)°, V = 2990.3(3) $Å^3$, Z = 4, T = 100(2) K, $2\theta_{max}$= 57.418°, D_{calc} (g cm^{-3}) = 2.335, $F(000)$ = 1976, μ (mm^{-1}) = 12.158, 42585 reflections collected, 7622 unique reflections (R_{int} = 0.0468, R_{sig} = 0.0298), 7273 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.108, T_{max} = 0.218, 327 refined parameters, 42 restraints, Good of Fit = S = 1.130, $R1$ = 0.0155, $wR2$ = 0.0366 (all data R = 0.0170, $wR2$ = 0.0370), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.794, $\Delta\rho_{min}$= -0.802 (e $Å^{-3}$).

Table S6. Crystal data and structure refinement for **AB_190918 (PzPbCl)**.

Identification code	**AB_190918**	
Empirical formula	C12 H38 Cl10 N6 O Pb2	
Formula weight	1051.36	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.3763(7) Å	a= 90°.
	b = 17.0747(8) Å	b= 96.283(2)°.
	c = 13.1719(7) Å	g = 90°.
Volume	2990.3(3) $Å^3$	
Z	4	
Density (calculated)	2.335 Mg/m^3	
Absorption coefficient	12.158 mm^{-1}	
F(000)	1976	
Crystal size	0.330 x 0.270 x 0.180 mm^3	
Theta range for data collection	2.591 to 28.709°.	
Index ranges	-18<=h<=18, -23<=k<=23, -17<=l<=17	
Reflections collected	42585	
Independent reflections	7622 [R(int) = 0.0468]	
Completeness to theta = 25.242°	98.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.218 and 0.108	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7622 / 42 / 327	

Goodness-of-fit on F^2	1.130
Final R indices [I>2sigma(I)]	R1 = 0.0155, wR2 = 0.0366
R indices (all data)	R1 = 0.0170, wR2 = 0.0370
Extinction coefficient	n/a
Largest diff. peak and hole	0.794 and -0.802 e.$Å^{-3}$

Table S7. Bond lengths [Å] and angles [°] for **AB_190918 (PzPbCl)**.

Pb(1)-Cl(2)	2.7532(6)
Pb(1)-Cl(1)	2.7667(6)
Pb(1)-Cl(5)	2.8081(5)
Pb(1)-Cl(3)	2.89488(15)
Pb(1)-Cl(3')#1	2.916(7)
Pb(1)-Cl(3')	2.930(7)
Pb(1)-Cl(6)	2.9791(6)
Pb(1)-Cl(4)	3.0110(6)
Pb(2)-Cl(9)	2.8014(5)
Pb(2)-Cl(11)	2.8023(5)
Pb(2)-Cl(10)	2.8127(5)
Pb(2)-Cl(8)	2.8647(5)
Pb(2)-Cl(6)	2.9312(6)
Pb(2)-Cl(7)	3.03005(16)
Cl(3)-Pb(1)#1	2.89486(15)
Cl(3')-Cl(3')#1	0.808(15)
Cl(3')-Pb(1)#1	2.916(7)
Cl(7)-Pb(2)#2	3.03004(17)
N(1)-C(3)	1.486(3)
N(1)-C(2)	1.491(3)
N(1)-H(1C)	0.9100
N(1)-H(1D)	0.9100
N(2)-C(1)	1.503(3)
N(2)-C(4)	1.507(3)
N(2)-C(5)	1.515(3)
N(2)-H(1N)	0.79(3)
N(3)-C(6)	1.487(3)
N(3)-H(3C)	0.9100
N(3)-H(3D)	0.9100
N(3)-H(3E)	0.9100
C(1)-C(2)	1.522(3)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-H(2A)	0.9900

C(2)-H(2B)	0.9900
C(3)-C(4)	1.509(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.512(3)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
N(4)-C(9)	1.487(3)
N(4)-C(8)	1.491(3)
N(4)-H(4C)	0.9100
N(4)-H(4D)	0.9100
N(5)-C(10)	1.507(3)
N(5)-C(7)	1.508(3)
N(5)-C(11)	1.512(3)
N(5)-H(2N)	0.84(3)
C(7)-C(8)	1.511(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.507(3)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12')	1.431(6)
C(11)-C(12)	1.578(5)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-N(6)	1.470(5)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900

N(6)-H(6C)	0.9100
N(6)-H(6D)	0.9100
N(6)-H(6E)	0.9100
C(12')-N(6')	1.508(8)
C(12')-H(12C)	0.9900
C(12')-H(12D)	0.9900
N(6')-H(6'1)	0.9100
N(6')-H(6'2)	0.9100
N(6')-H(6'3)	0.9100
O(1)-H(1E)	0.89
O(1)-H(1F)	0.8750

Cl(2)-Pb(1)-Cl(1)	87.286(19)
Cl(2)-Pb(1)-Cl(5)	89.131(16)
Cl(1)-Pb(1)-Cl(5)	82.589(16)
Cl(2)-Pb(1)-Cl(3)	89.430(14)
Cl(1)-Pb(1)-Cl(3)	175.778(14)
Cl(5)-Pb(1)-Cl(3)	94.714(11)
Cl(2)-Pb(1)-Cl(3')#1	94.48(15)
Cl(1)-Pb(1)-Cl(3')#1	176.08(15)
Cl(5)-Pb(1)-Cl(3')#1	100.92(16)
Cl(2)-Pb(1)-Cl(3')	84.41(15)
Cl(1)-Pb(1)-Cl(3')	167.91(14)
Cl(5)-Pb(1)-Cl(3')	88.50(16)
Cl(3')#1-Pb(1)-Cl(3')	15.9(3)
Cl(2)-Pb(1)-Cl(6)	92.663(17)
Cl(1)-Pb(1)-Cl(6)	86.317(17)
Cl(5)-Pb(1)-Cl(6)	168.667(17)
Cl(3)-Pb(1)-Cl(6)	96.492(12)
Cl(3')#1-Pb(1)-Cl(6)	90.11(16)
Cl(3')-Pb(1)-Cl(6)	102.80(16)
Cl(2)-Pb(1)-Cl(4)	171.631(16)
Cl(1)-Pb(1)-Cl(4)	92.713(18)
Cl(5)-Pb(1)-Cl(4)	82.573(15)
Cl(3)-Pb(1)-Cl(4)	90.150(12)
Cl(3')#1-Pb(1)-Cl(4)	86.05(15)

Cl(3')-Pb(1)-Cl(4)	94.23(15)
Cl(6)-Pb(1)-Cl(4)	95.689(16)
Cl(9)-Pb(2)-Cl(11)	79.861(15)
Cl(9)-Pb(2)-Cl(10)	95.071(16)
Cl(11)-Pb(2)-Cl(10)	96.758(17)
Cl(9)-Pb(2)-Cl(8)	91.632(16)
Cl(11)-Pb(2)-Cl(8)	91.698(15)
Cl(10)-Pb(2)-Cl(8)	170.013(16)
Cl(9)-Pb(2)-Cl(6)	96.889(16)
Cl(11)-Pb(2)-Cl(6)	176.434(16)
Cl(10)-Pb(2)-Cl(6)	84.947(17)
Cl(8)-Pb(2)-Cl(6)	86.908(16)
Cl(9)-Pb(2)-Cl(7)	164.380(11)
Cl(11)-Pb(2)-Cl(7)	84.879(11)
Cl(10)-Pb(2)-Cl(7)	89.988(12)
Cl(8)-Pb(2)-Cl(7)	85.469(11)
Cl(6)-Pb(2)-Cl(7)	98.273(12)
Pb(1)#1-Cl(3)-Pb(1)	180.0
Cl(3')#1-Cl(3')-Pb(1)#1	83.0(10)
Cl(3')#1-Cl(3')-Pb(1)	81.1(10)
Pb(1)#1-Cl(3')-Pb(1)	164.1(3)
Pb(2)-Cl(6)-Pb(1)	168.95(2)
Pb(2)#2-Cl(7)-Pb(2)	180.0
C(3)-N(1)-C(2)	111.39(17)
C(3)-N(1)-H(1C)	109.3
C(2)-N(1)-H(1C)	109.3
C(3)-N(1)-H(1D)	109.3
C(2)-N(1)-H(1D)	109.3
H(1C)-N(1)-H(1D)	108.0
C(1)-N(2)-C(4)	108.93(16)
C(1)-N(2)-C(5)	113.67(16)
C(4)-N(2)-C(5)	109.25(16)
C(1)-N(2)-H(1N)	110(2)
C(4)-N(2)-H(1N)	110(2)
C(5)-N(2)-H(1N)	105(2)
C(6)-N(3)-H(3C)	109.5

C(6)-N(3)-H(3D)	109.5
H(3C)-N(3)-H(3D)	109.5
C(6)-N(3)-H(3E)	109.5
H(3C)-N(3)-H(3E)	109.5
H(3D)-N(3)-H(3E)	109.5
N(2)-C(1)-C(2)	110.40(16)
N(2)-C(1)-H(1A)	109.6
C(2)-C(1)-H(1A)	109.6
N(2)-C(1)-H(1B)	109.6
C(2)-C(1)-H(1B)	109.6
H(1A)-C(1)-H(1B)	108.1
N(1)-C(2)-C(1)	111.49(17)
N(1)-C(2)-H(2A)	109.3
C(1)-C(2)-H(2A)	109.3
N(1)-C(2)-H(2B)	109.3
C(1)-C(2)-H(2B)	109.3
H(2A)-C(2)-H(2B)	108.0
N(1)-C(3)-C(4)	110.91(18)
N(1)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3A)	109.5
N(1)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	108.0
N(2)-C(4)-C(3)	110.04(17)
N(2)-C(4)-H(4A)	109.7
C(3)-C(4)-H(4A)	109.7
N(2)-C(4)-H(4B)	109.7
C(3)-C(4)-H(4B)	109.7
H(4A)-C(4)-H(4B)	108.2
C(6)-C(5)-N(2)	115.46(18)
C(6)-C(5)-H(5A)	108.4
N(2)-C(5)-H(5A)	108.4
C(6)-C(5)-H(5B)	108.4
N(2)-C(5)-H(5B)	108.4
H(5A)-C(5)-H(5B)	107.5
N(3)-C(6)-C(5)	114.10(18)

N(3)-C(6)-H(6A)	108.7
C(5)-C(6)-H(6A)	108.7
N(3)-C(6)-H(6B)	108.7
C(5)-C(6)-H(6B)	108.7
H(6A)-C(6)-H(6B)	107.6
C(9)-N(4)-C(8)	110.22(18)
C(9)-N(4)-H(4C)	109.6
C(8)-N(4)-H(4C)	109.6
C(9)-N(4)-H(4D)	109.6
C(8)-N(4)-H(4D)	109.6
H(4C)-N(4)-H(4D)	108.1
C(10)-N(5)-C(7)	110.00(16)
C(10)-N(5)-C(11)	110.17(17)
C(7)-N(5)-C(11)	112.03(18)
C(10)-N(5)-H(2N)	107.2(18)
C(7)-N(5)-H(2N)	107.4(18)
C(11)-N(5)-H(2N)	109.9(18)
N(5)-C(7)-C(8)	110.81(18)
N(5)-C(7)-H(7A)	109.5
C(8)-C(7)-H(7A)	109.5
N(5)-C(7)-H(7B)	109.5
C(8)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	108.1
N(4)-C(8)-C(7)	109.49(19)
N(4)-C(8)-H(8A)	109.8
C(7)-C(8)-H(8A)	109.8
N(4)-C(8)-H(8B)	109.8
C(7)-C(8)-H(8B)	109.8
H(8A)-C(8)-H(8B)	108.2
N(4)-C(9)-C(10)	110.30(18)
N(4)-C(9)-H(9A)	109.6
C(10)-C(9)-H(9A)	109.6
N(4)-C(9)-H(9B)	109.6
C(10)-C(9)-H(9B)	109.6
H(9A)-C(9)-H(9B)	108.1
N(5)-C(10)-C(9)	111.07(18)

N(5)-C(10)-H(10A)	109.4
C(9)-C(10)-H(10A)	109.4
N(5)-C(10)-H(10B)	109.4
C(9)-C(10)-H(10B)	109.4
H(10A)-C(10)-H(10B)	108.0
C(12')-C(11)-N(5)	116.3(3)
N(5)-C(11)-C(12)	113.4(2)
N(5)-C(11)-H(11A)	108.9
C(12)-C(11)-H(11A)	108.9
N(5)-C(11)-H(11B)	108.9
C(12)-C(11)-H(11B)	108.9
H(11A)-C(11)-H(11B)	107.7
N(6)-C(12)-C(11)	114.2(3)
N(6)-C(12)-H(12A)	108.7
C(11)-C(12)-H(12A)	108.7
N(6)-C(12)-H(12B)	108.7
C(11)-C(12)-H(12B)	108.7
H(12A)-C(12)-H(12B)	107.6
C(12)-N(6)-H(6C)	109.5
C(12)-N(6)-H(6D)	109.5
H(6C)-N(6)-H(6D)	109.5
C(12)-N(6)-H(6E)	109.5
H(6C)-N(6)-H(6E)	109.5
H(6D)-N(6)-H(6E)	109.5
C(11)-C(12')-N(6')	109.1(5)
C(11)-C(12')-H(12C)	109.9
N(6')-C(12')-H(12C)	109.9
C(11)-C(12')-H(12D)	109.9
N(6')-C(12')-H(12D)	109.9
H(12C)-C(12')-H(12D)	108.3
C(12')-N(6')-H(6'1)	109.5
C(12')-N(6')-H(6'2)	109.5
H(6'1)-N(6')-H(6'2)	109.5
C(12')-N(6')-H(6'3)	109.5
H(6'1)-N(6')-H(6'3)	109.5
H(6'2)-N(6')-H(6'3)	109.5

H(1E)-O(1)-H(1F) 107.4

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1 #2 -x,-y,-z

Table S8. Torsion angles [°] for **AB_190918 (PzPbCl)**.

C(4)-N(2)-C(1)-C(2)	-58.5(2)
C(5)-N(2)-C(1)-C(2)	179.47(17)
C(3)-N(1)-C(2)-C(1)	-54.1(2)
N(2)-C(1)-C(2)-N(1)	55.9(2)
C(2)-N(1)-C(3)-C(4)	55.7(2)
C(1)-N(2)-C(4)-C(3)	60.2(2)
C(5)-N(2)-C(4)-C(3)	-175.14(17)
N(1)-C(3)-C(4)-N(2)	-59.0(2)
C(1)-N(2)-C(5)-C(6)	-59.5(2)
C(4)-N(2)-C(5)-C(6)	178.58(18)
N(2)-C(5)-C(6)-N(3)	-71.0(2)
C(10)-N(5)-C(7)-C(8)	56.1(2)
C(11)-N(5)-C(7)-C(8)	179.04(19)
C(9)-N(4)-C(8)-C(7)	60.2(2)
N(5)-C(7)-C(8)-N(4)	-58.7(2)
C(8)-N(4)-C(9)-C(10)	-59.6(2)
C(7)-N(5)-C(10)-C(9)	-55.2(2)
C(11)-N(5)-C(10)-C(9)	-179.22(19)
N(4)-C(9)-C(10)-N(5)	57.2(2)
C(10)-N(5)-C(11)-C(12')	-159.6(3)
C(7)-N(5)-C(11)-C(12')	77.6(4)
C(10)-N(5)-C(11)-C(12)	-123.6(2)
C(7)-N(5)-C(11)-C(12)	113.6(2)
N(5)-C(11)-C(12)-N(6)	-77.5(3)
N(5)-C(11)-C(12')-N(6')	73.1(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1 #2 -x,-y,-z