

Supporting Information for

A one-dimensional dual emissive hybrid perovskite with flexibly tunable white-light emission

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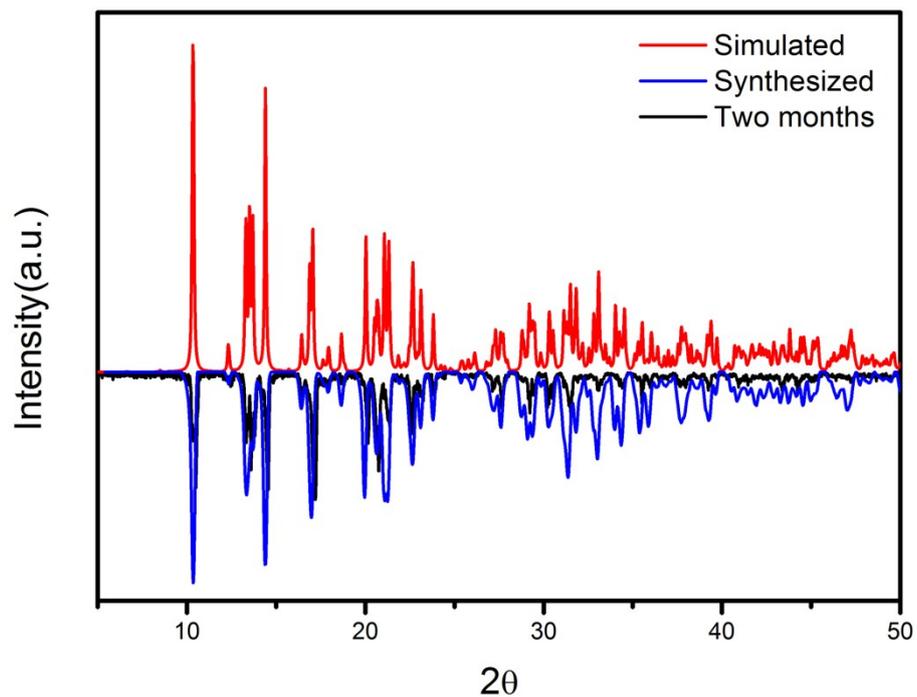


Figure S1. Powder X-ray diffraction patterns of original synthesized NAPC.

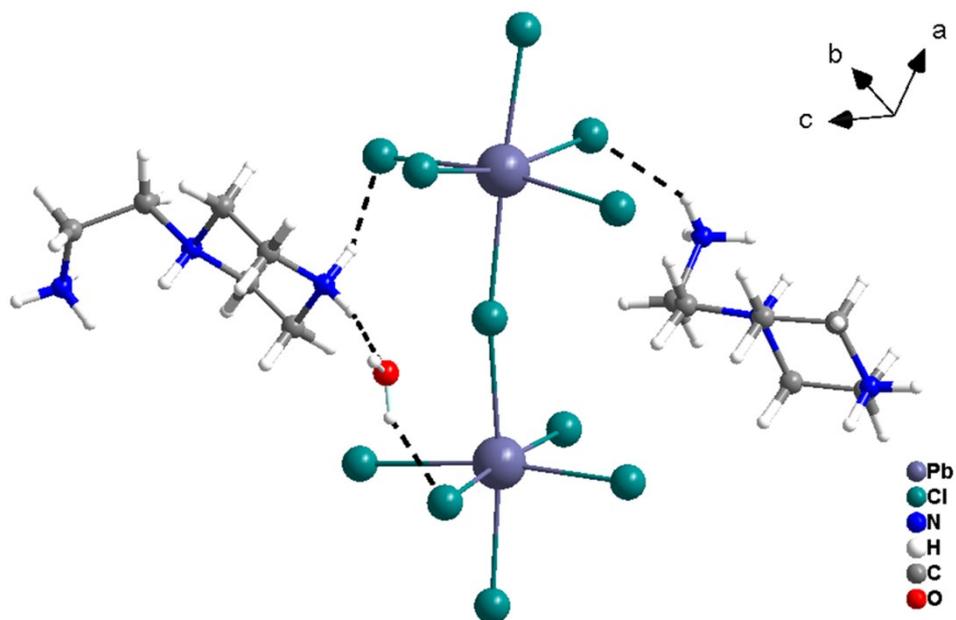


Figure S2. Hydrogen bonds in the compound NAPC, and the asymmetric unit consists of NAPC (In order to clearly express the hydrogen bond, some hydrogen atoms are removed.).

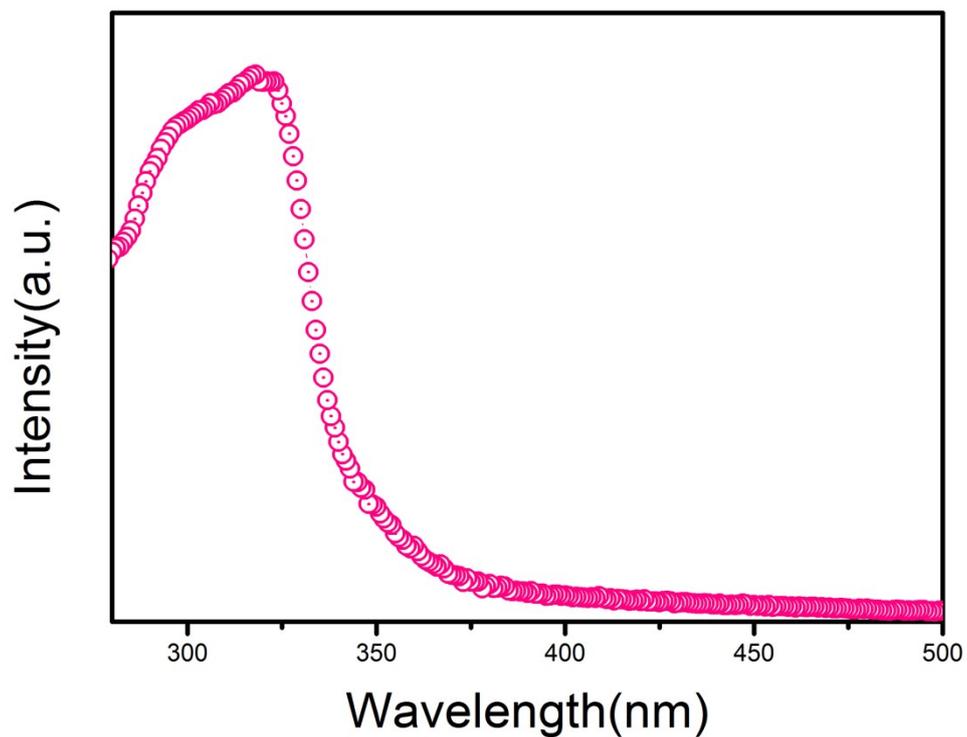


Figure S3. UV-vis absorption spectra of NAPC.

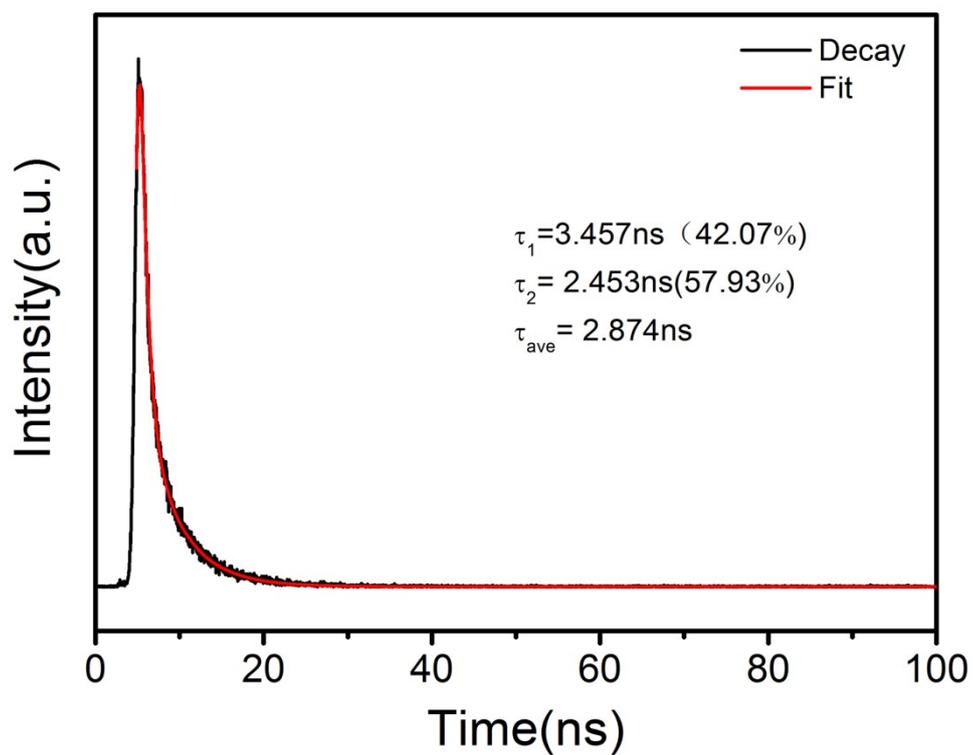


Figure S4. Photoluminescence decay and fitting curves of (N-AEP)Cl₃ at 402 nm.

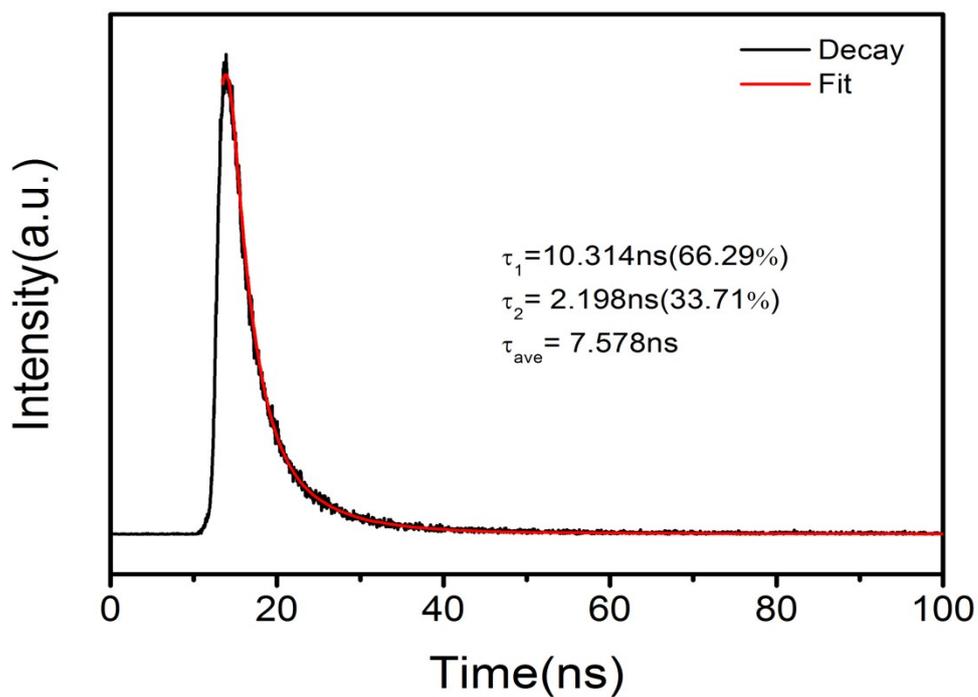


Figure S5. Photoluminescence decay and fitting curves of NAPC at 396 nm.

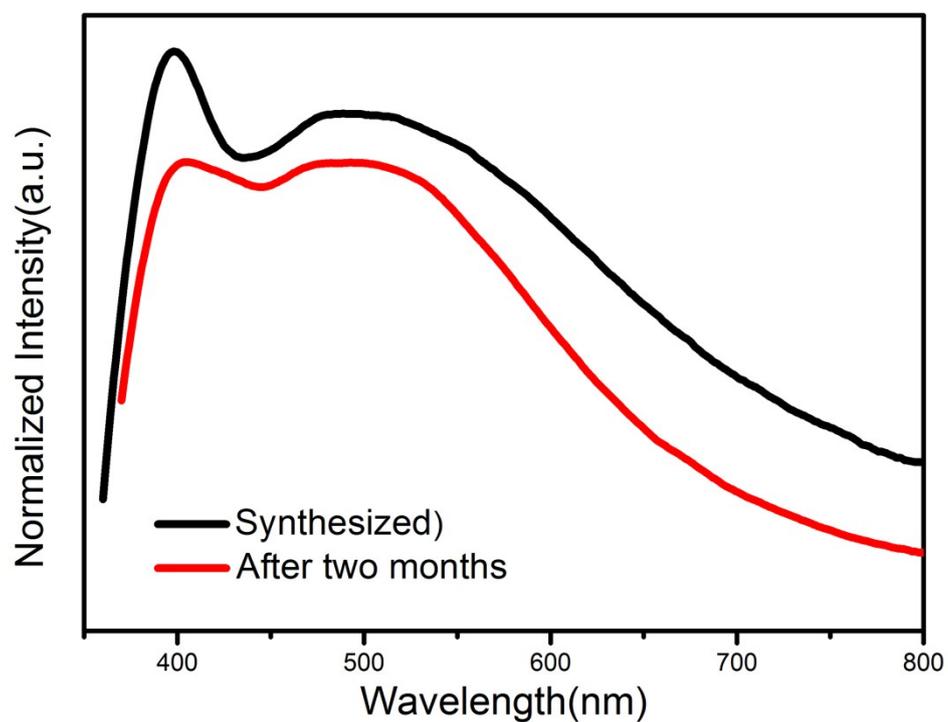


Figure S6. Emission spectra of the crystal of compound NAPC original synthesized and that exposed to ambient condition for two months.

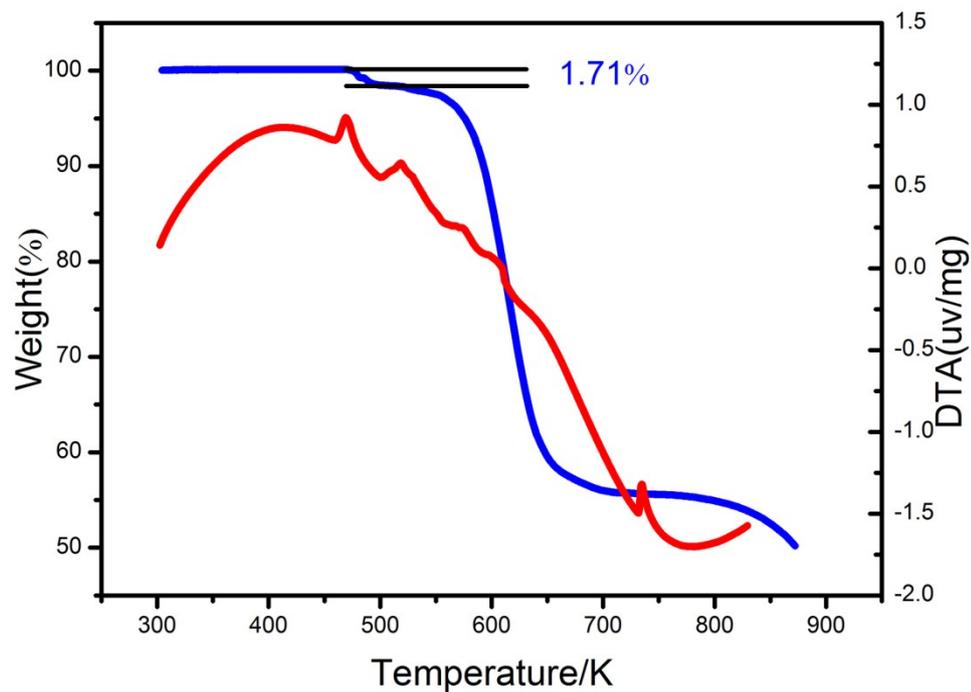


Figure S7. DTA and thermogravimetric curves for NAPC.

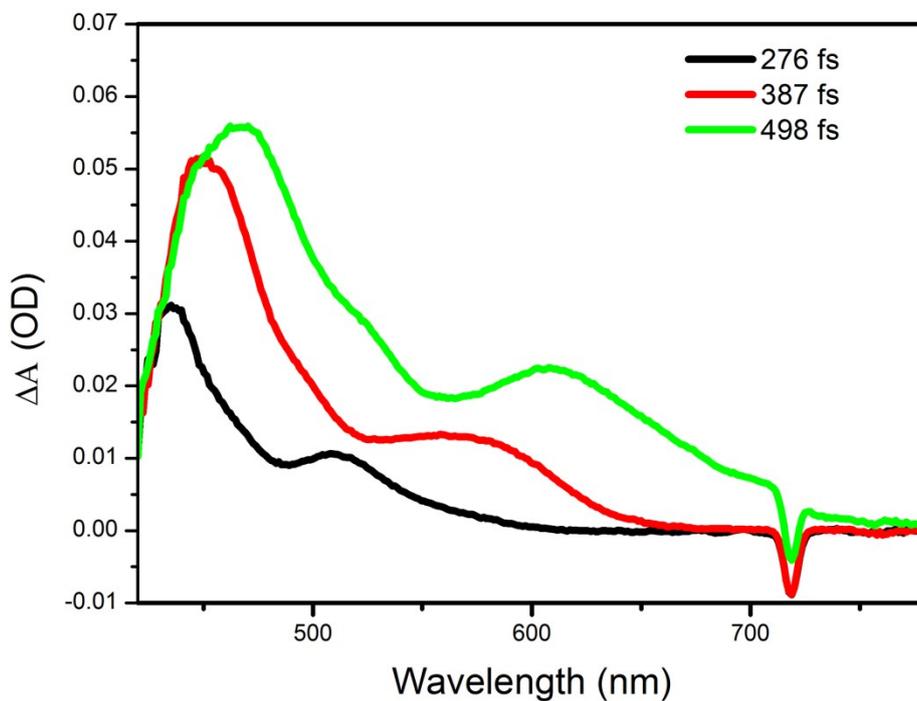


Figure S8. Details of transient (TA) absorption for NAPC excited by 360 nm wavelength laser. optical density. Photo-induced absorption is observed throughout the whole visible spectrum. The irregular peaks located at ~ 720 nm are from frequency doubling of the light source.

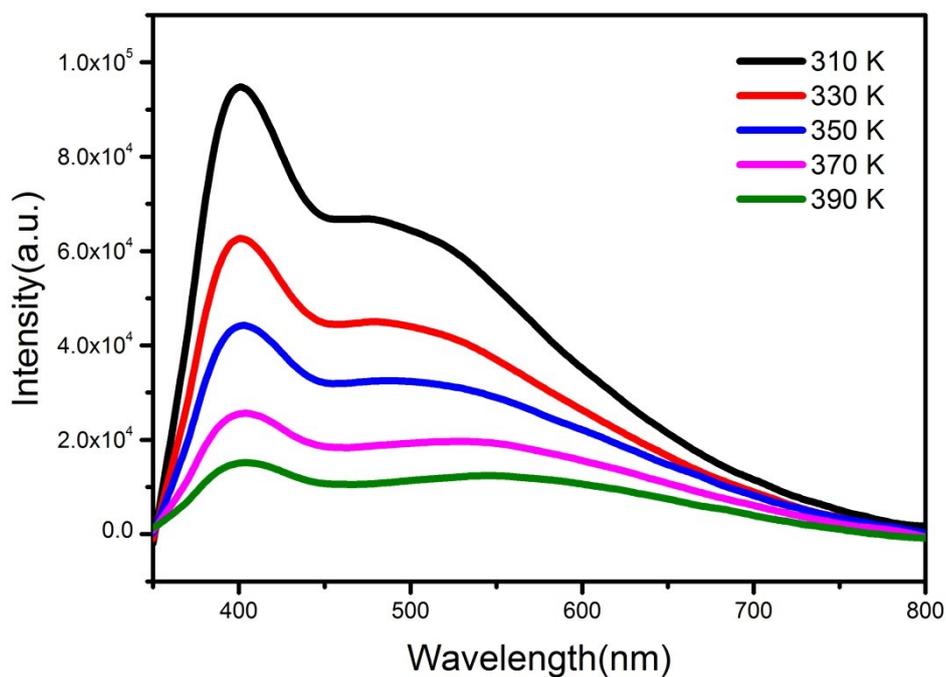


Figure S9. Emission spectra of compound NAPC at different temperatures.

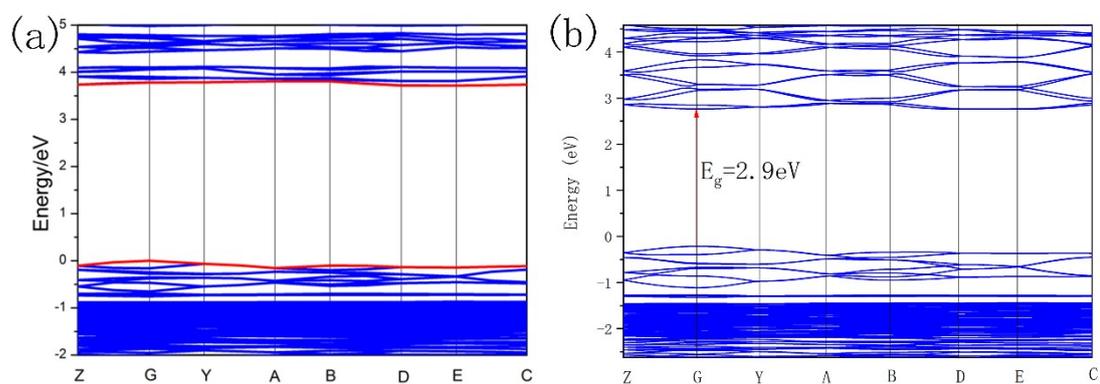


Figure S10. calculated band gap of NAPC. (a) without spin-orbit coupling, 3.7 eV, (b) with spin-orbit coupling, 2.9 eV.

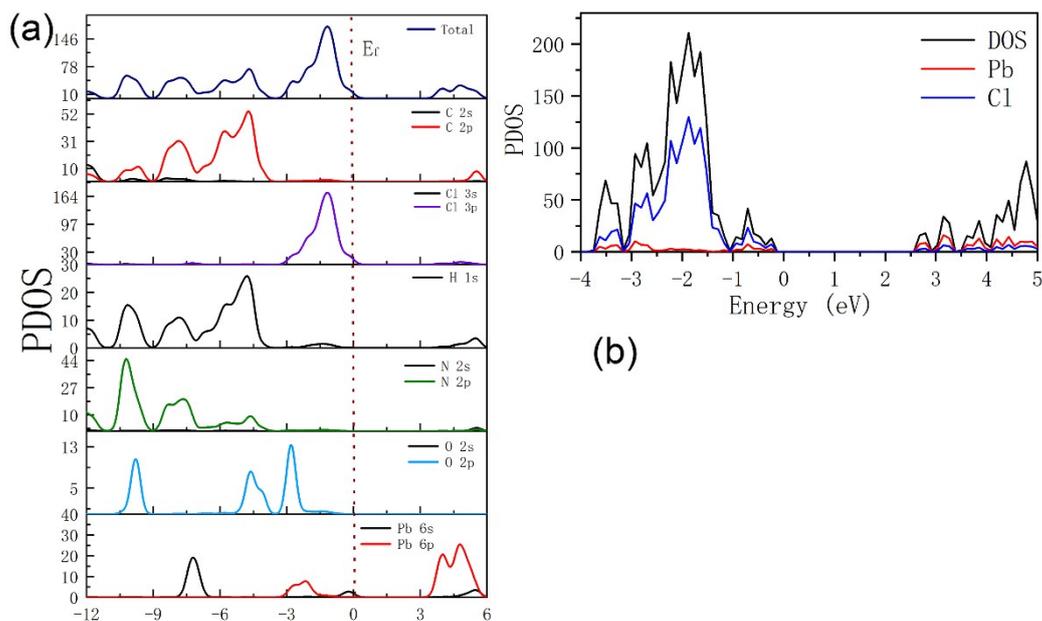


Figure S11. Partial density of states. (a) without spin-orbit coupling (SOC), (b) with SOC.

Table S1. Crystal Data and Structure Refinement for **NAPC**

Empirical formula	$C_{12}H_{38}Cl_{10}N_6OPb_2$
Formula weight	1051.36
Temperature/K	100 (2)
Space group	$P2_1/c$
$a/\text{\AA}$	13.3797 (3)
$b/\text{\AA}$	17.0669 (3)
$c/\text{\AA}$	13.1789 (3)
$\alpha/^\circ$	90.00
$\beta/^\circ$	96.323 (2)
$\gamma/^\circ$	90.00
Volume/ \AA^3	2991.09 (11)
Z	4
$\rho_{\text{calc}}/\text{g/cm}^3$	2.335
μ/mm^{-1}	12.155
F(000)	1976.0
Radiation	Mo $K\alpha$ ($\lambda = 0.71073$)
2 θ range for data collection/ $^\circ$	6.98 to 52.74

Index ranges	-16 ≤ h ≤ 15, -21 ≤ k ≤ 21, -14 ≤ l ≤ 16
Reflections collected	18228
Independent reflections	6071 [R _{int} = 0.0526]
Data/restraints/parameters	6071/32/287
Goodness-of-fit on F ²	1.082
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0372, wR ₂ = 0.0912
Final R indexes [all data]	R ₁ = 0.0412, wR ₂ = 0.0939
Largest diff. peak/hole / e Å ⁻³	2.90/-3.35

Table S2. The Pb–Cl bond lengths of **NAPC**

Bond	(Å)	Bond	(Å)
Pb(1)– Cl(1)	2.8037(16)	Pb(2)– Cl(6)	2.9780(18)
Pb(1)– Cl(2)	3.0308(2)	Pb(2)– Cl(7)	2.7647(17)
Pb(1)– Cl(3)	2.8625(16)	Pb(2)– Cl(8)	3.0134(17)
Pb(1)– Cl(4)	2.8022(16)	Pb(2)– Cl(9)	2.8965(2)
Pb(1)– Cl(5)	2.8138(16)	Pb(2)– Cl(10)	2.7512(18)
Pb(1)– Cl(6)	2.9324(18)	Pb(2)– Cl(11)	2.8095(15)

Table S3 Hydrogen bond lengths and bond angles

Bond	d(D-H)	d(H...A)	d(D..A)	D-H...A
N(1)-H(1A)..Cl(5)	0.92	2.36	3.228(5)	158
N(1)-H(1B)..O(1)	0.92	1.8	2.782(7)	165
N(2)-H(2)..Cl(7) ^{#3}	0.93	2.54	3.304(5)	130
N(2)-H(2)..Cl(11) ^{#3}	0.93	2.54	3.304(5)	139
N(3)-H(3C)..Cl(9) ^{#4}	0.91	2.54	3.396(9)	157
N(3)-H(3D)..Cl(8) ^{#5}	0.91	2.24	3.059(9)	150
N(3)-H(3E)..Cl(7) ^{#3}	0.91	2.16	3.035(9)	161
N(4)-H(4C)..O(1) ^{#6}	0.92	1.90	2.817(7)	174
N(4)-H(4D)..Cl(3) ^{#6}	0.92	2.35	3.157(6)	147
N(5)-H(5)..Cl(1) ^{#7}	0.93	2.59	3.304(5)	134
N(5)-H(5)..Cl(4) ^{#7}	0.93	2.48	3.210(6)	135
N(6)-H(6C)..Cl(4)	0.91	2.35	3.160(5)	148

N(6)-H(6D)..Cl(11) ^{#1}	0.91	2.29	3.180(5)	165
N(6)-H(6E)..Cl(1) ^{#7}	0.91	2.29	3.188(5)	169
O(1)-H(13)..Cl(1) ^{#2}	0.83	2.27	3.069(6)	162
O(1)-H(14)..Cl(7)	0.87	2.31	3.059(6)	144
C(2)--H(2A)..Cl(5)	0.99	2.73	3.543(7)	140
C(2)--H(2B)..Cl(10) ^{#4}	0.99	2.78	3.728(7)	161
C(2)--H(2B)..Cl(7) ^{#3}	0.99	2.73	3.246(7)	113
C(3)--H(3A)..Cl(3) ^{#2}	0.99	2.75	3.433(7)	127
C(5)--H(5A)..Cl(11) ^{#4}	0.99	2.82	3.758(8)	158
C(6)--H(6A)..Cl(11) ^{#3}	0.99	2.81	3.692(9)	148
C(6)--H(6B)..Cl(6) ^{#5}	0.99	2.66	3.634(9)	169
C(7)--H(7B)..Cl(1) ^{#7}	0.99	2.68	3.406(7)	131
C(10)--H(10A)..Cl(3)	0.99	2.78	3.633(7)	144
C(11)--H(11A)..Cl(10)	0.99	2.75	3.657(7)	152
C(11)--H(11B)..Cl(3)	0.99	2.83	3.655(7)	142

Symmetry transformations used to generate equivalent atoms:

[#1] = 1-x, -y, -z [#2] = 2-x, -y, 1-z [#3] = 1-x, -y, 1-z [#4] = 1-x, 1/2+y, 1/2-z
[#5] = x, 1/2-y, 1/2+z [#6] = x, -1/2-y, -1/2+z [#7] = 2-x, -y, -z