Electronic Supplementary Material (ESI)

A facile synthesis of two new IR optical perovskites based on 1,4-diazabicyclo[2,2,2]octane with high laser damage threshold

Jun-Ling Song,[a] Wen-Jun Chen,[a] Kai-Bin Chu,[a] and Yu-Hua Zhou[b*]

[a]International Joint Research Center for Photoresponsive Molecules and Materials, School of Chemical and Material Engineering, Jiangnan University, Wuxi 214122, China

[b]School of Materials Science and Engineering, Nanyang Technological University, Singapore 639798, Singapore. *Corresponding author: yzhou@uclan.ac.uk

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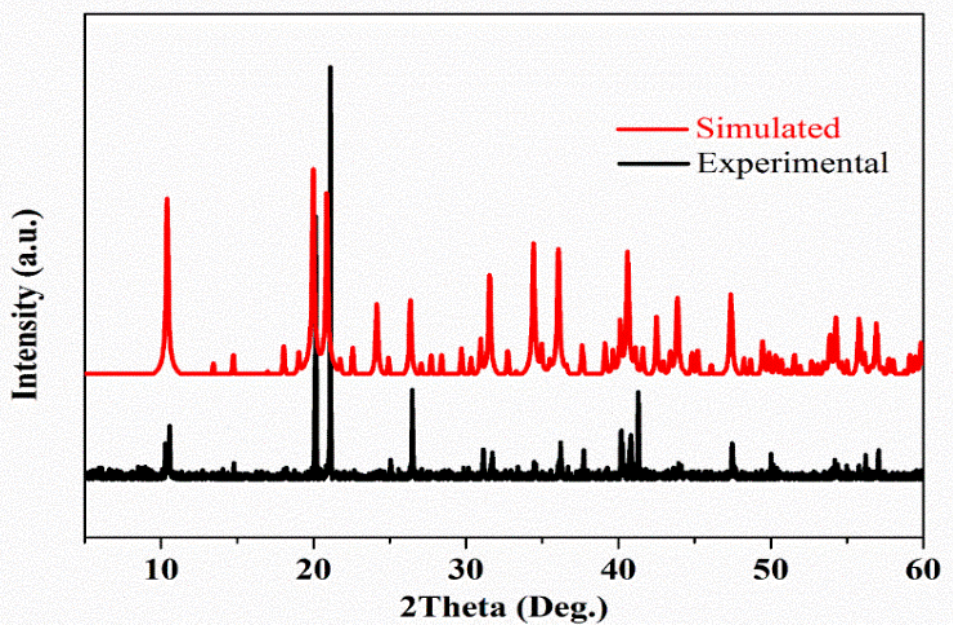
(a)


Simulated
Experimental
Intensity (a.u.)
10
20
30
40
50
60
2Theta (Deg.)

(b)

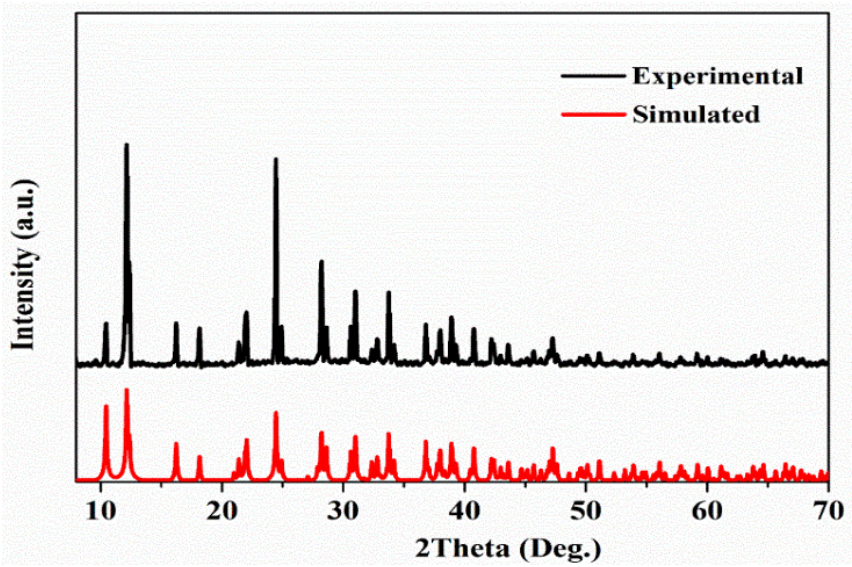
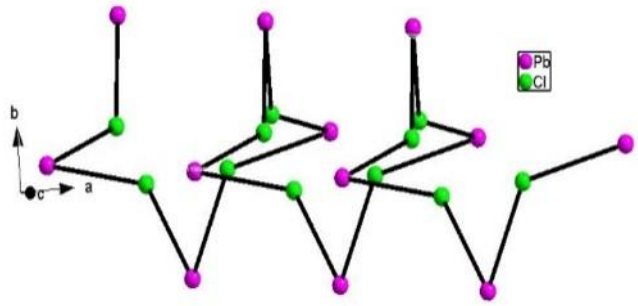

Experimental
Simulated
Intensity (a.u.)
10
20
30
40
50
60
70
2Theta (Deg.)

Fig. S1.

(a)



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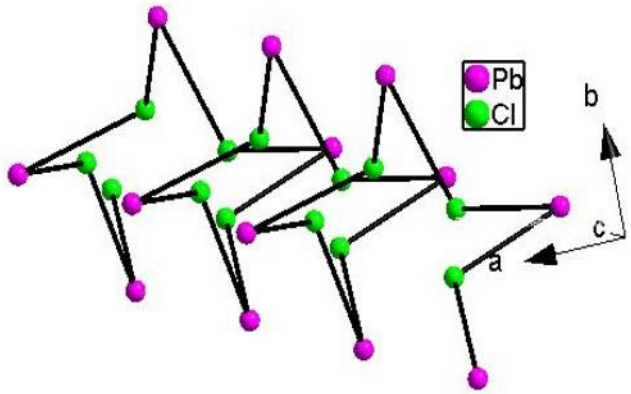


(c)

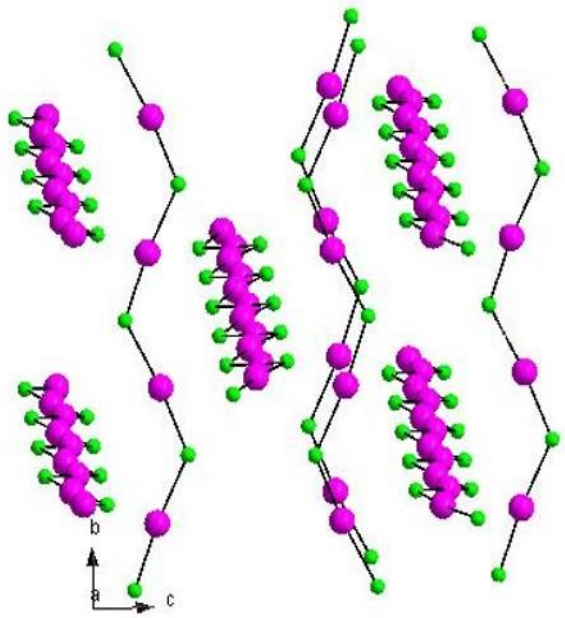
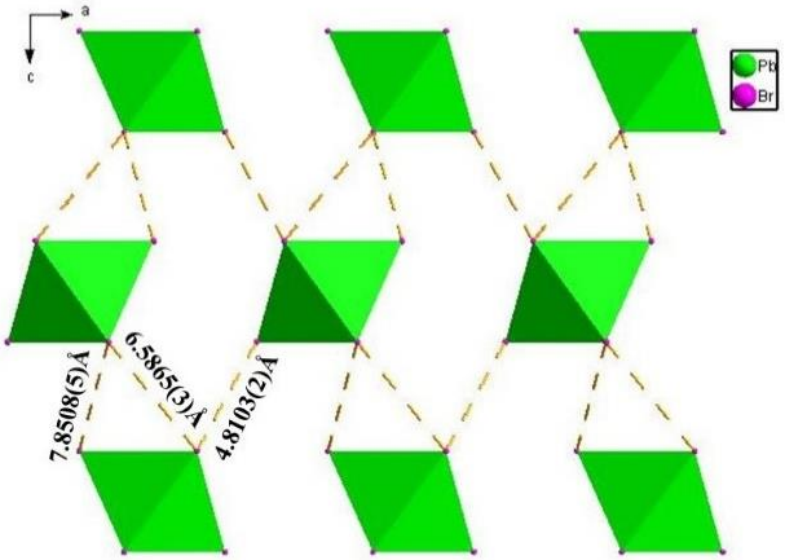


Fig S2.

(a)



(b)

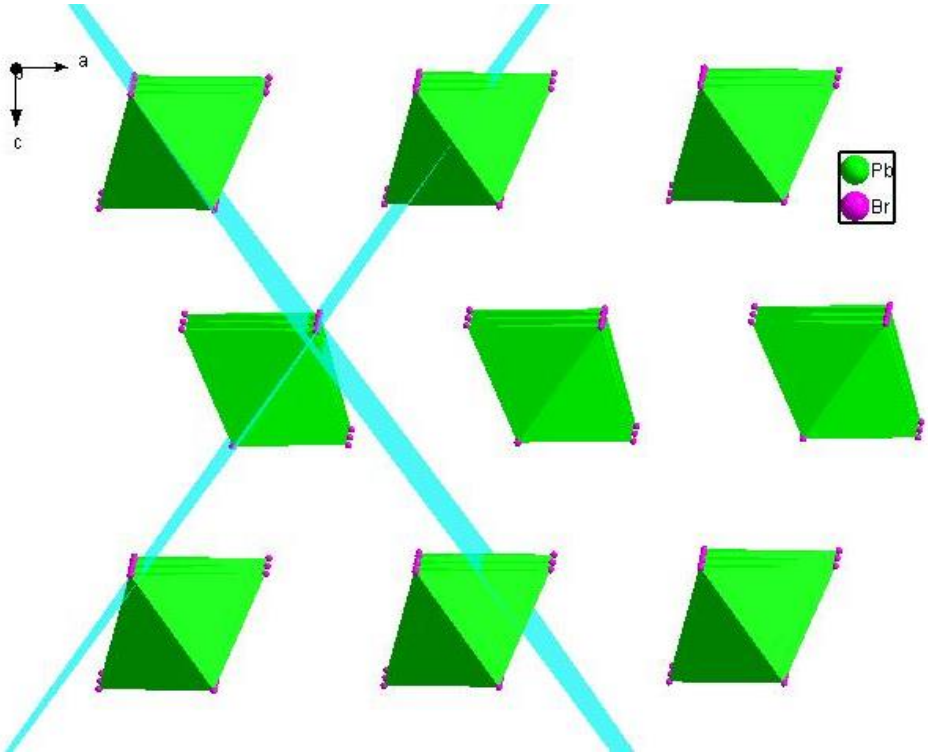
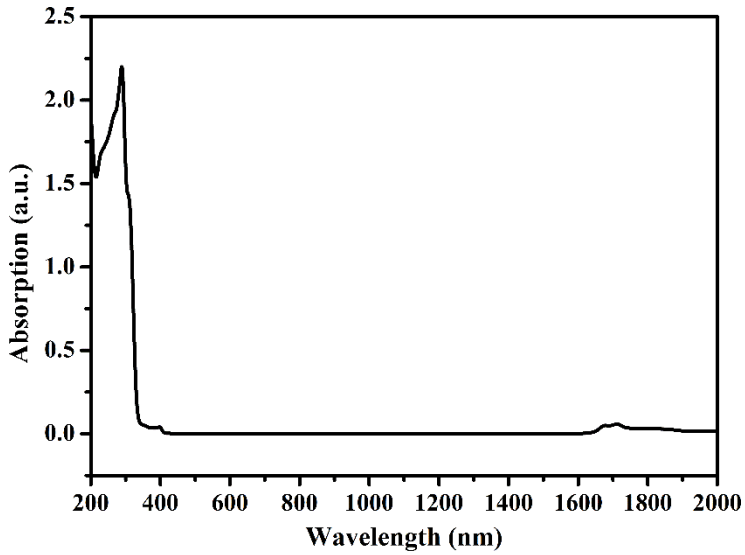


Fig. S3.

(a)


Absorption (a.u.)
Wavelength (nm)
2.5
2.0
1.5
1.0
0.5
0.0
200
400
600
800
1000
1200
1400
1600
1800
2000

(b)

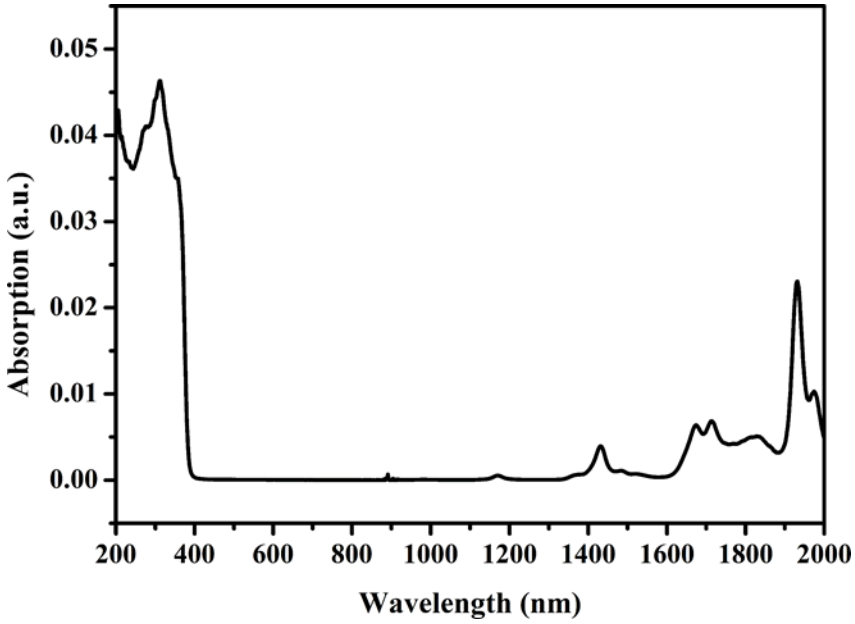
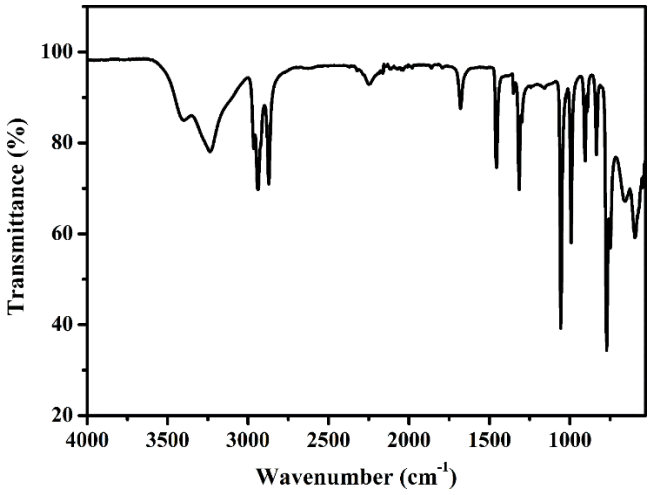
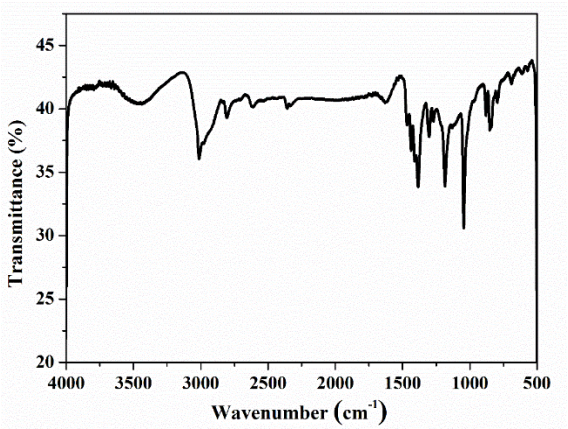

Absorption (a.u.)
Wavelength (nm)
0.05
0.04
0.03
0.02
0.01
0.00
200
400
600
800
1000
1200
1400
1600
1800
2000

Fig. S4.

(a)


Transmittance (%)
100
80
60
40
20
4000
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)

(b)


Transmittance (%)
45
40
35
30
25
20
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

(c)

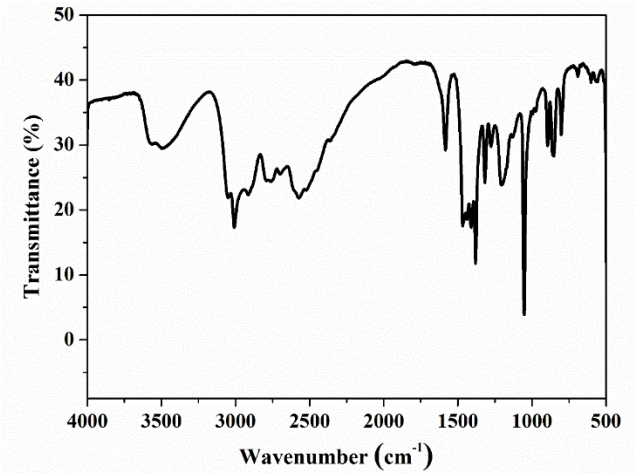

Transmittance (%)
50
40
30
20
10
0
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

Fig. S5.

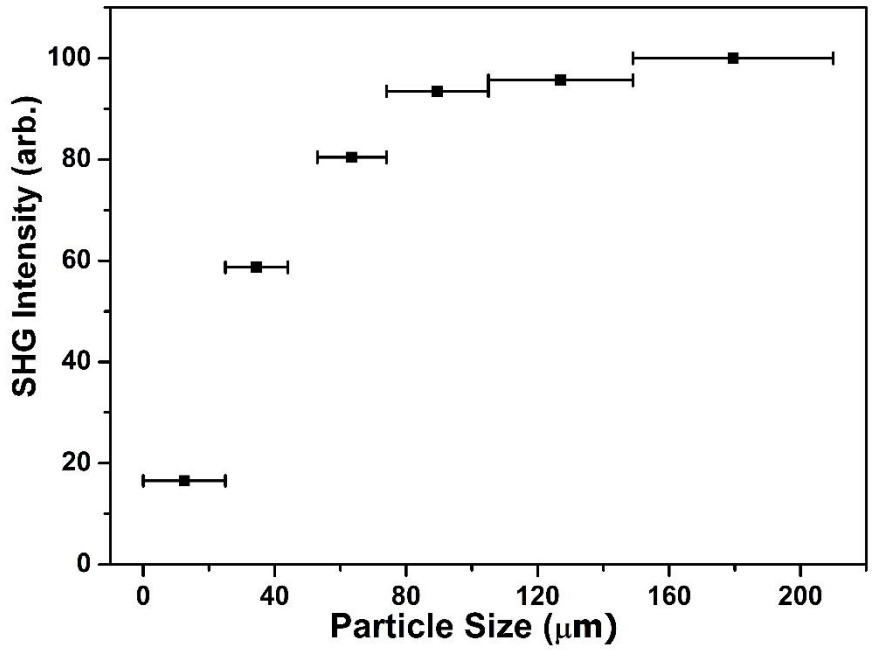

SHG Intensity (arb.)
100
80
60
40
20
0
0
40
80
120
160
200
Particle Size (μm)

Fig. S6.

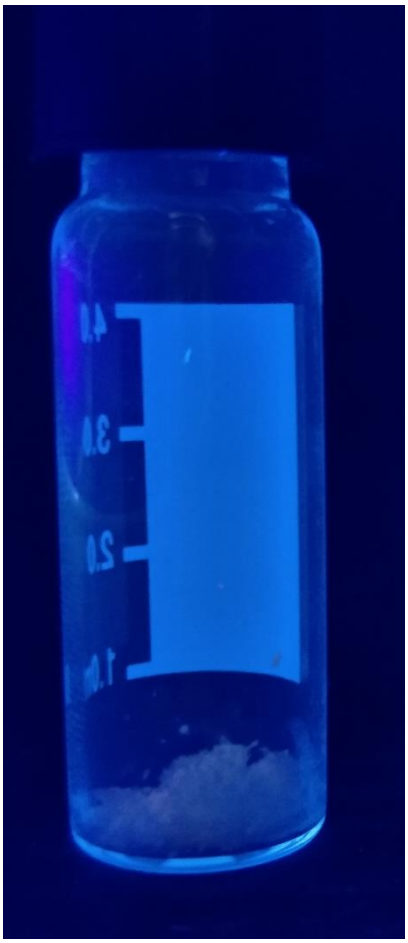


Fig. S7.

Table S1.

Compound **1**				
	x	y	z	U(eq)
Pb(1)	9827(1)	2533(1)	1135(1)	17(1)
Cl(2)	10420(3)	420(3)	0	39(1)
Cl(3)	7339(2)	2206(3)	456(2)	40(1)
Cl(1)	9336(3)	664(3)	2500	48(1)
N(1)	7619(11)	2855(12)	8321(7)	61(3)
C(2)	6333(10)	2285(12)	8243(7)	38(3)
C(3)	7852(18)	3903(18)	7761(9)	83(6)
C(1)	8701(13)	1907(13)	7910(10)	55(4)
Cl(4)	9166(3)	4947(3)	2048(2)	35(1)
Compound **2**				
	x	y	z	U(eq)
Pb(1)	16667	23333	-10522(1)	22(1)
Br(1)	15316(2)	20631(3)	-9202(2)	52(1)
N(1)	16667	23333	-5600(30)	27(7)
N(2)	16667	23333	-7410(30)	34(10)
Br(2)	13505(5)	21752(3)	-11604(3)	72(1)
C(1)	14980(30)	22488(15)	-5954(19)	36(5)
C(2)	15010(30)	22505(16)	-7035(18)	51(8)
O(1W)	16667	23333	-3730(30)	64(15)

Table S2

Pb(1)-Cl(3)	2.798(2)	N(1)-C(3)	1.389(17)
Pb(1)-Cl(2)	2.8305(16)	N(1)-C(2)	1.470(15)
Pb(1)-Cl(1)	2.8426(16)	N(1)-C(1)	1.616(17)
Pb(1)-Cl(4)#1	2.897(2)	N(1)-Cl(3)#6	3.225(10)
Pb(1)-Cl(4)	2.933(3)	N(1)-Cl(4)#7	3.399(11)
Pb(1)-Cl(3)#2	2.951(2)	C(2)-C(3)#8	1.504(17)
Cl(2)-Pb(1)#3	2.8305(16)	C(3)-C(2)#8	1.504(17)
Cl(3)-Pb(1)#4	2.951(2)	C(1)-C(1)#8	1.50(3)
Cl(1)-Pb(1)#5	2.8426(16)	Cl(4)-Pb(1)#9	2.897(2)
Cl(3)-Pb(1)-Cl(2)	84.10(8)	Cl(4)#1-Pb(1)-Cl(4)	83.35(6)
Cl(3)-Pb(1)-Cl(1)	90.12(8)	Cl(3)-Pb(1)-Cl(3)#2	173.82(4)
Cl(2)-Pb(1)-Cl(1)	85.58(8)	Cl(2)-Pb(1)-Cl(3)#2	98.35(7)
Cl(3)-Pb(1)-Cl(4)#1	81.92(8)	Cl(1)-Pb(1)-Cl(3)#2	84.43(7)
Cl(2)-Pb(1)-Cl(4)#1	87.95(7)	Cl(4)#1-Pb(1)-Cl(3)#2	103.79(8)
Cl(1)-Pb(1)-Cl(4)#1	170.22(6)	Cl(4)-Pb(1)-Cl(3)#2	85.52(8)
Cl(3)-Pb(1)-Cl(4)	92.87(8)	Pb(1)#3-Cl(2)-Pb(1)	133.39(14)
Cl(2)-Pb(1)-Cl(4)	171.12(6)	Pb(1)-Cl(3)-Pb(1)#4	130.45(9)
Cl(1)-Pb(1)-Cl(4)	102.81(8)	Pb(1)#5-Cl(1)-Pb(1)	138.16(17)

Symmetry transformations used to generate equivalent atoms: #1 -y+3/2,x-1/2,z-1/4; #2 x+1/2,-y+1/2,-z+1/4; #3 y+1,x-1,-z; #4 x-1/2,-y+1/2,-z+1/4; #5 -y+1,-x+1,-z+1/2; #6 x,y,z+1;#7 -y+3/2,x-1/2,z+3/4; #8 -y+1,-x+1,-z+3/2; #9 y+1/2,-x+3/2,z+1/4.

Table S3

Pb(1)-Br(1)#1	2.959(3)	N(1)-C(1)#1	1.51(3)
Pb(1)-Br(1)	2.959(3)	N(1)-C(1)	1.51(3)
Pb(1)-Br(1)#2	2.959(3)	N(1)-C(1)#2	1.51(3)
Pb(1)-Br(2)#1	3.084(4)	N(1)-O(1W)	2.67(6)
Pb(1)-Br(2)#2	3.084(4)	N(2)-C(2)#1	1.49(3)
Pb(1)-Br(2)	3.084(4)	N(2)-C(2)#2	1.49(3)
Br(1)-N(2)	3.43(4)	N(2)-C(2)	1.49(3)
C(1)-C(2)	1.54(3)	O(1W)-Br(1)#3	3.414(8)
Br(1)#1-Pb(1)-Br(1)	83.75(9)	Br(1)#1-Pb(1)-Br(2)	170.48(11)
Br(1)#1-Pb(1)-Br(1)#2	83.75(9)	Br(1)-Pb(1)-Br(2)	89.18(8)
Br(1)-Pb(1)-Br(1)#2	83.75(9)	Br(1)#2-Pb(1)-Br(2)	89.18(8)
Br(1)#1-Pb(1)-Br(2)#1	89.18(8)	Br(2)#1-Pb(1)-Br(2)	97.10(13)
Br(1)-Pb(1)-Br(2)#1	89.18(8)	Br(2)#2-Pb(1)-Br(2)	97.10(13)
Br(1)#2-Pb(1)-Br(2)#1	170.48(11)	Pb(1)-Br(1)-N(2)	87.9(5)
Br(1)#1-Pb(1)-Br(2)#2	89.18(8)	Br(1)#2-Pb(1)-Br(2)#2	89.18(8)
Br(1)-Pb(1)-Br(2)#2	170.48(11)	Br(2)#1-Pb(1)-Br(2)#2	97.10(13)

Symmetry transformations used to generate equivalent atoms: #1 -y+4,x-y+3,z; #2 -x+y+1,-x+4,z; #3 -x+3,-y+4,z+1/2.