Electronic Supplementary Material for CrystEngComm

Supporting Inormtion

Structural Diversity and Retro-Crystal Engineering Analysis of Iodometalate hybrids

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Table S1. Crystal data and structure refinement for $(NC(CH_2)_2NH_3)_2PbI_4$.

Identification code	PbCNC2
Empirical formula	C6 H14 I4 N4 Pb
Formula weight	857.00
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pnma
Unit cell dimensions	a = 8.6370(4) A alpha = 90 deg.
	b = 20.346(2) A beta = 90 deg.
	c = 9.7847(5) A gamma = 90 deg.
Volume	1719.5(2) A^3
Z, Calculated density	4, 3.311 Mg/m^3
Absorption coefficient	16.977 mm^-1
F(000)	1488
Crystal size	0.276 x 0.106 x 0.088 mm
Theta range for data collection	3.66 to 30.02 deg.
Limiting indices	-12<=h<=10, -28<=k<=28, -13<=l<=13
Reflections collected / unique	26269 / 2514 [R(int) = 0.0505]
Completeness to theta = 30.02	97.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.2727 and 0.0894
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2514 / 0 / 75
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0332, wR2 = 0.0522
R indices (all data)	R1 = 0.0667, wR2 = 0.0581
Extinction coefficient	0.00015(3)
Largest diff. peak and hole	1.426 and -1.250 e.A^-3

Table S2. Bond lengths [A] and angles [deg] for $(NC(CH_2)_2NH_3)_2PbI_4$.

Pb(1)-I(2)	3.1648(6)	N(1)-H(1C)	0.8900
Pb(1)-I(3)	3.1738(6)	N(1)-H(1D)	0.8900
Pb(1)-I(1)	3.1831(5)	N(1)-H(1E)	0.8900
Pb(1)-I(1)#1	3.1831(5)	C(2)-C(3)	1.479(9)
Pb(1)-I(2)#2	3.3522(6)	C(2)-C(1)	1.503(8)
Pb(1)-I(3)#3	3.3692(6)	C(2)-H(2A)	0.9700
I(3)-Pb(1)#4	3.3692(6)	C(2)-H(2B)	0.9700
I(2)-Pb(1)#5	3.3522(6)	C(1)-H(1A)	0.9700
N(2)-C(3)	1.182(8)	C(1)-H(1B)	0.9700
N(1)-C(1)	1.482(8)		
I(2)-Pb(1)-I(3)	93.133(16)	C(1)-N(1)-H(1D)	109.5
I(2)-Pb(1)-I(1)	94.680(11)	H(1C)-N(1)-H(1D)	109.5
I(3)-Pb(1)-I(1)	90.518(11)	C(1)-N(1)-H(1E)	109.5
I(2)-Pb(1)-I(1)#1	94.680(11)	H(1C)-N(1)-H(1E)	109.5
I(3)-Pb(1)-I(1)#1	90.518(10)	H(1D)-N(1)-H(1E)	109.5
I(1)-Pb(1)-I(1)#1	170.513(17)	C(3)-C(2)-C(1)	112.2(5)
I(2)-Pb(1)-I(2)#2	83.271(8)	C(3)-C(2)-H(2A)	109.2
I(3)-Pb(1)-I(2)#2	176.404(16)	C(1)-C(2)-H(2A)	109.2
I(1)-Pb(1)-I(2)#2	89.779(10)	C(3)-C(2)-H(2B)	109.2
I(1)#1-Pb(1)-I(2)#2	89.779(10)	C(1)-C(2)-H(2B)	109.2
I(2)-Pb(1)-I(3)#3	175.830(16)	H(2A)-C(2)-H(2B)	107.9
I(3)-Pb(1)-I(3)#3	82.696(8)	N(1)-C(1)-C(2)	111.6(5)
I(1)-Pb(1)-I(3)#3	85.389(10)	N(1)-C(1)-H(1A)	109.3
I(1)#1-Pb(1)-I(3)#3	85.389(10)	C(2)-C(1)-H(1A)	109.3
I(2)#2-Pb(1)-I(3)#3	100.899(15)	N(1)-C(1)-H(1B)	109.3
Pb(1)-I(3)-Pb(1)#4	177.59(2)	C(2)-C(1)-H(1B)	109.3
Pb(1)-I(2)-Pb(1)#5	174.64(2)	H(1A)-C(1)-H(1B)	108.0
C(1)-N(1)-H(1C)	109.5	N(2)-C(3)-C(2)	177.0(7)

Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2,z #2 x-1/2,y,-z-1/2 #3 x-1/2,y,-z+1/2 #4 x+1/2,y,-z+1/2 #5 x+1/2,y,-z-1/2

Table S3. Anisotropic displacement parameters for $(NC(CH_2)_2NH_3)_2PbI_4$.

The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pb(1)	24(1)	26(1)	27(1)	0	0(1)	0
I(3)	27(1)	46(1)	31(1)	0	-7(1)	0
I(2)	29(1)	46(1)	39(1)	0	12(1)	0
I(1)	45(1)	28(1)	34(1)	0(1)	-1(1)	1(1)
N(2)	60(4)	68(4)	40(3)	-7(3)	-14(3)	-22(3)
N(1)	65(4)	69(5)	25(2)	-2(3)	-3(3)	-20(4)
C(2)	54(4)	34(4)	29(3)	2(3)	-4(3)	-21(3)
C(1)	51(4)	37(4)	47(4)	-12(3)	-1(3)	0(3)
C(3)	50(4)	54(5)	18(3)	4(3)	0(3)	8(4)

Table S4. Hydrogen bonds for $(NC(CH_2)_2NH_3)_2PbI_4$ [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1C)...N(2)#6	0.89	1.97	2.847(9)	169.2
N(1)-H(1D)...I(1)#4	0.89	2.94	3.630(5)	135.4
N(1)-H(1E)...I(1)#7	0.89	2.88	3.663(6)	147.4

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z #2 x-1/2,y,-z-1/2 #3 x-1/2,y,-z+1/2

#4 x+1/2,y,-z+1/2 #5 x+1/2,y,-z-1/2 #6 -x,-y,-z

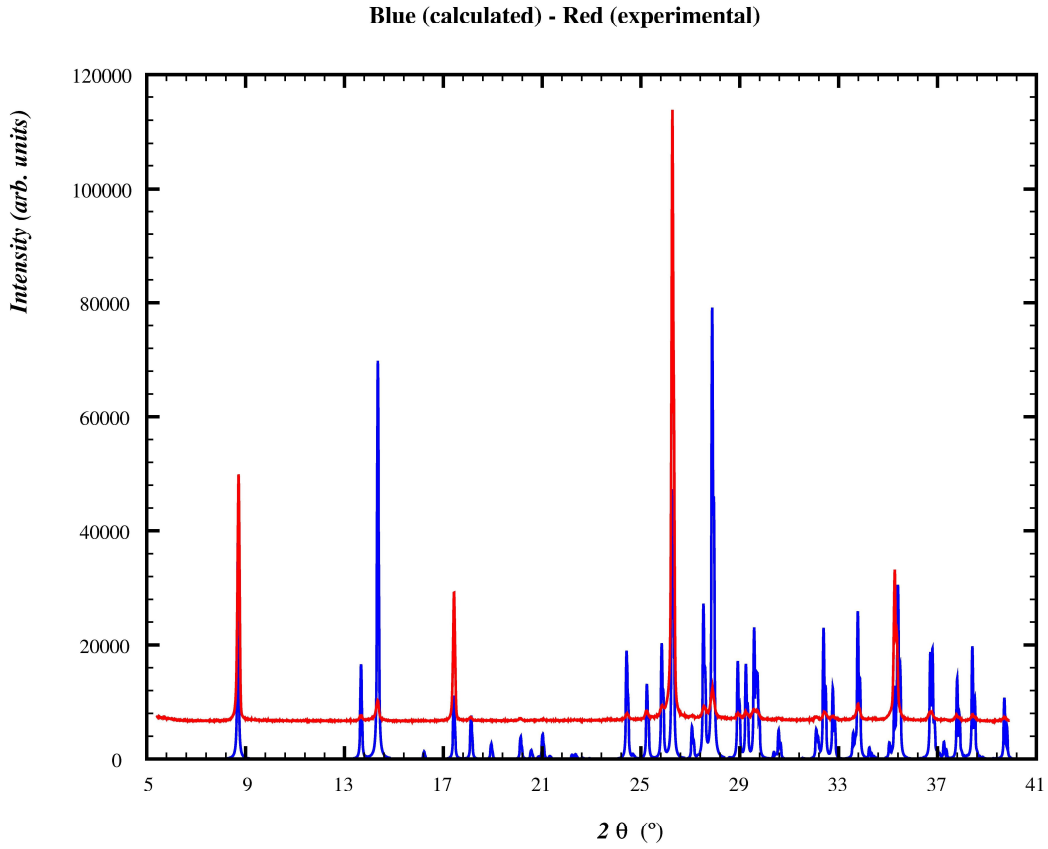
#7 x+1,y,z

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for $(NC(CH_2)_2NH_3)_2PbI_4$.

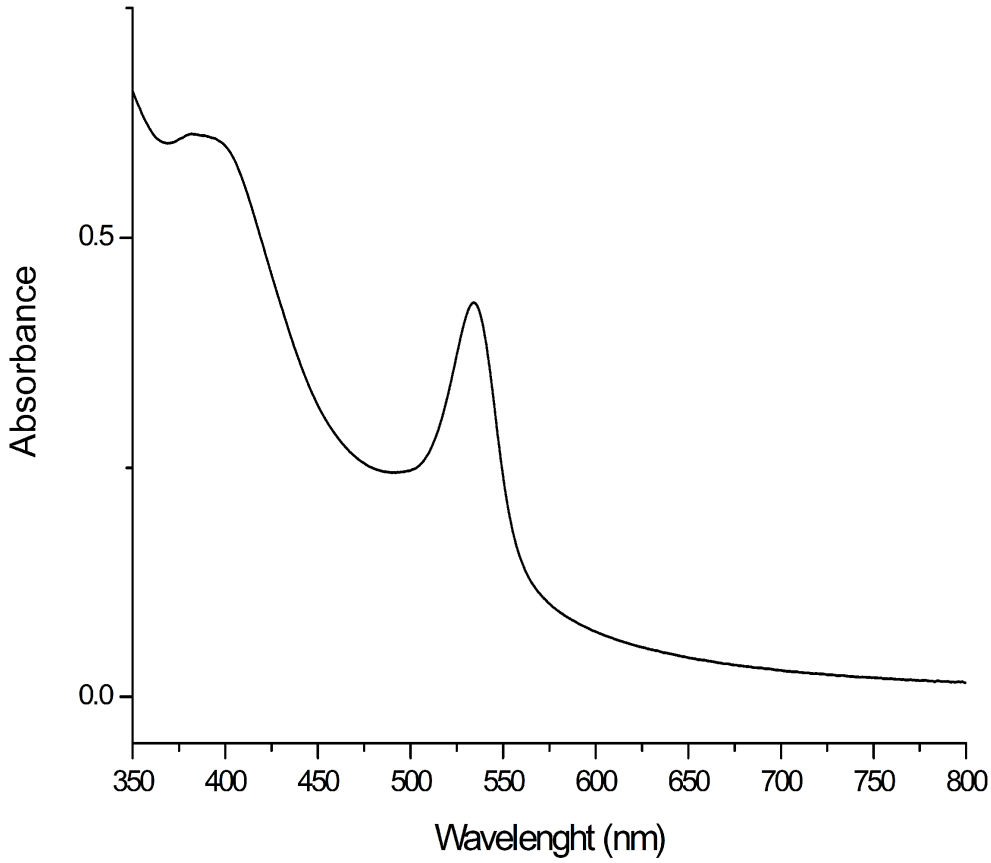
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pb(1)	-3225(1)	2500	-11(1)	26(1)
I(3)	-740(1)	2500	2379(1)	35(1)
I(2)	-665(1)	2500	-2325(1)	38(1)
I(1)	-3471(1)	941(1)	148(1)	36(1)
N(2)	-28(7)	46(3)	-1703(6)	56(2)
N(1)	2477(7)	864(3)	1241(4)	53(2)
C(2)	2131(8)	952(3)	-1257(5)	39(2)
C(1)	1945(8)	1288(3)	102(6)	45(2)
C(3)	904(8)	460(4)	-1509(5)	41(2)

The X-ray Powder Pattern for $(NC(CH_2)_2NH_3)_2PbI_4$:



The UV/Vis spectrum for $(NC(CH_2)_2NH_3)_2PbI_4$:



checkCIF/PLATON report (publication check) for $(NC(CH_2)_2NH_3)_2PbI_4$

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Bond precision: C-C = 0.0090 A Wavelength=0.71073
Cell: a=8.6370(4) b=20.346(2) c=9.7847(5)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1719.5(2)	1719.5(2)
Space group	P n m a	Pnma
Hall group	-P 2ac 2n	-P_2ac_2n
Moiety formula	I4 Pb, 2(C3 H7 N2)	I4 Pb, 2(C3 H7 N2)
Sum formula	C6 H14 I4 N4 Pb	C6 H14 I4 N4 Pb
Mr	857.01	857.01
Dx,g cm-3	3.310	3.311
Z	4	4
Mu (mm-1)	16.976	16.977
F000	1488.0	1488.0
F000'	1468.36	
h,k,lmax	12,28,13	12,28,13
Nref	2576	2514
Tmin,Tmax	0.133,0.224	0.089,0.273
Tmin'	0.008	

Correction method= AbsCorr=MULTI-SCAN
Data completeness= Ratio = 0.976 Theta(max)= 30.020
R(reflections)= 0.0332(1675) wR2(reflections)= 0.0581(2514)
S = 1.024 Npar= 75

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT112_ALERT_2_B ADDSYM Detects Additional (Pseudo) Symm. Elem.. B
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Pb1 --I1 .. 10.19 su

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Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.Absorption correction given as multi-scan
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.98
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Pb1--I2 .. .84 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Pb1--I3 . 9.76 su
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang 9
PLAT062_ALERT_4_C Rescale T(min) & T(max) by 0.82
PLAT147_ALERT_1_C su on Symmetry Constrained Cell Angle(s) .....?
PLAT194_ALERT_1_C Missing _cell_measurement_reflns_used datum ...?
PLAT195_ALERT_1_C Missing _cell_measurement_theta_max datum ....?
PLAT196_ALERT_1_C Missing _cell_measurement_theta_min datum ...?
PLAT764_ALERT_4_C Overcomplete CIF Bond List Detected (Rep/Expd)1.20 Ratio

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Alert level G

ABSTM02_ALERT_3_G When printed, the submitted absorption T values will be replaced by the scaled T values. Since the ratio of scaled T's is identical to the ratio of reported T values, the scaling does not imply a change to the absorption corrections used in the study.
Ratio of Tmax expected/reported 0.823
Tmax scaled 0.224
Tmin scaled 0.074
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature 293K
PLAT200_ALERT_1_G Check the Reported _diffrn_ambient_temperature 293K

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0 ALERT level A = In general: serious problem
2 ALERT level B = Potentially serious problem
11 ALERT level C = Check and explain
3 ALERT level G = General alerts; check

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
