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Synthesis, Characterization, and Electronic Structures of Organically Templated Lead Halides with One- and Two-Dimensional Hybrid Structures, $[(nbq)(PbI_3)]_n$ and $\{[(CH_3)_3NC_2H_4N(CH_3)_3]_3(Pb_6I_{18})\}_n$

Organically Templated Lead Halides

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Original cell in Angstroms and degrees:

8.051 14.060 16.544 90.00 90.00 90.00

14295 Reflections read from file shelxl.hkl; mean (I/sigma) = 7.93

Lattice exceptions: P A B C I F Obv Rev All

N (total) =	0	7117	7139	7152	7124	10704	9566	9544	14295
N (int>3sigma) =	0	4217	4361	4428	4253	6503	5834	5833	8701
Mean intensity =	0.0	109.2	108.7	112.3	107.7	110.1	110.3	109.7	108.8
Mean int/sigma =	0.0	7.9	7.9	8.2	7.8	8.0	8.0	8.0	7.9

Lattice type: P chosen Volume: 1872.80

DETERMINATION OF REDUCED (NIGGLI) CELL

Transformation from original cell (HKLF-matrix):
1.0000 0.0000 0.0000 0.0000 1.0000 0.0000 0.0000 0.0000 1.0000

Unitcell: 8.051 14.060 16.544 90.00 90.00 90.00

Niggli form: a.a = 64.82 b.b = 197.68 c.c = 273.71
b.c = 0.00 a.c = 0.00 a.b = 0.00

SEARCH FOR HIGHER METRIC SYMMETRY

Option A: FOM = 0.000 deg. ORTHORHOMBIC P-lattice R(int) = 0.059 [11886]
Cell: 8.051 14.060 16.544 90.00 90.00 90.00 Volume: 1872.80
Matrix: 1.0000 0.0000 0.0000 0.0000 1.0000 0.0000 0.0000 0.0000 1.0000

Option A selected

SPACE GROUP DETERMINATION

Lattice exceptions: P A B C I F Obv Rev All

N (total) =	0	7117	7139	7152	7124	10704	9566	9544	14295
N (int>3sigma) =	0	4217	4361	4428	4253	6503	5834	5833	8701
Mean intensity =	0.0	109.2	108.7	112.3	107.7	110.1	110.3	109.7	108.8
Mean int/sigma =	0.0	7.9	7.9	8.2	7.8	8.0	8.0	8.0	7.9

Crystal system O and Lattice type P selected

Mean |E*E-1| = 0.799 [expected .968 centrosym and .736 non-centrosym]

Chiral flag NOT set

Systematic absence exceptions:

	b--	c--	n--	21--	-c-	-a-	-n-	-21-	--a	--b	--n	--21
N	595	584	569	0	234	238	230	0	224	211	207	0
N I>3s	423	421	288	0	134	113	137	0	110	120	140	0
<I>	234.8	243.4	74.7	0.0	161.7	66.7	158.0	0.0	50.3	201.7	205.3	0.0
<I/s>	11.3	11.3	6.7	0.0	9.2	6.8	9.4	0.0	7.3	10.8	11.5	0.0

Option	Space Group	No.	Type	Axes	CSD	R(int)	N(eq)	Syst. Abs.	CFOM
[A]	P222	# 16	chiral	1	14	0.059	11886	0.0 / 6.7	8.54
[B]	Pmm2	# 25	non-cen	1	9	0.059	11886	0.0 / 6.7	11.88
[C]	Pmm2	# 25	non-cen	5	9	0.059	11886	0.0 / 6.7	11.88
[D]	Pmm2	# 25	non-cen	3	9	0.059	11886	0.0 / 6.7	11.88
[E]	Pmmm	# 47	centro	1	7	0.059	11886	0.0 / 6.7	16.85
[F]	P222(1)	# 17	chiral	1	26	0.059	11886	0.0 / 6.7	5.58
[G]	P222(1)	# 17	chiral	5	26	0.059	11886	0.0 / 6.7	5.58
[H]	P222(1)	# 17	chiral	3	26	0.059	11886	0.0 / 6.7	5.58
[I]	P2(1)2(1)2	# 18	chiral	1	359	0.059	11886	0.0 / 6.7	2.15

[J] P2(1)2(1)2 # 18 chiral 5 359 0.059 11886 0.0 / 6.7 2.15
[K] P2(1)2(1)2 # 18 chiral 3 359 0.059 11886 0.0 / 6.7 2.15
[L] P2(1)2(1)2(1) # 19 chiral 1 5917 0.059 11886 0.0 / 6.7 1.89

Option [L] chosen

Determination of unit-cell contents

Formula: C15 H30 N2 Pb2 I6

Formula weight = 1414.19

Tentative Z (number of formula units/cell) = 3.0 giving rho = 3.762,
non-H atomic volume = 25.0 and following cell contents and analysis:

C	45.00	12.74 %	H	90.00	2.14 %
N	6.00	1.98 %	I	18.00	53.84 %
Pb	6.00	29.30 %			

F(000) = 1848.0 Mo-K(alpha) radiation Mu (mm-1) = 20.89

File lihh.ins set up as follows:

```
TITL lihh in P2(1)2(1)2(1)
CELL 0.71073   8.0512  14.0599  16.5443  90.000  90.000  90.000
ZERR    3.00   0.0005   0.0011   0.0013   0.000   0.000   0.000
LATT -1
SYMM 0.5-X, -Y, 0.5+Z
SYMM -X, 0.5+Y, 0.5-Z
SYMM 0.5+X, 0.5-Y, -Z
SFAC C H N I PB
UNIT 45 90 6 18 6
TREF
HKLF 4
END
```

14295 Reflections written to new reflection file lihh.hkl
