Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

Crystal structures and optical properties of haloplumbates hybrids templated by in situ synthesized 1,4-diazabicyclo[2.2.2]octane derivatives

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Table S1. Crystal and structure refinement data for **1**−**6**.

	1	**2**	**3**
Formula	$(C_{16}H_{36}N_4)(PbI_6)$	$(C_{20}H_{44}N_4)(Pb_3I_{10})$	$(C_{24}H_{52}N_4)(Pb_3I_{10})$
Color and habit	colourless block	yellow rod	yellow rod
Crystal size (mm)	0.15 × 0.10 × 0.10	0.20 × 0.08 × 0.08	0.20 × 0.08 × 0.08
Crystal system	Cubic	Monoclinic	Monoclinic
Space group	*Pa*–3	$P2_1/c$	$P2_1/c$
a (Å)	14.6567(3)	9.3555(6)	10.839(4)
b (Å)	14.6567(3)	20.2788(12)	20.008(6)
c (Å)	14.6567(3)	14.7688(10)	12.216(4)
α (°)	90	90	90
β (°)	90	126.541(4)	110.346(3)
γ (°)	90	90	90
V (Å^3)	3148.54(11)	2251.1(2)	2483.9(14)
Z	4	2	2
Formula	1234.93	2231.19	2287.27

weight			
ρ_{calcd} (g cm^{-3})	2.605	3.292	3.058
μ (mm^{-1})	11.250	18.065	16.376
F(000)	2168	1936	2000
θ (°)	2.78–25.49	2.84–25.50	2.05–25.50
Completeness	0.999	0.990	0.997
Index ranges of measured data	$-17 \le h \le 17$, $-17 \le k \le 17$, $-17 \le l \le 17$,	$-11 \le h \le 11$, $-24 \le k \le 24$, $-17 \le l \le 14$,	$-12 \le h \le 13$, $-24 \le k \le 24$, $-14 \le l \le 14$,
Reflections measured	19929	16765	18127
Indep. reflections (R_{int})	986 (0.0403)	4150 (0.0553)	4595 (0.0664)
Obs. reflections [$I > 2\sigma(I)$]	985	3406	3616
R_1, wR_2 indices (obs.)	0.0296, 0.0760	0.0298, 0.0588	0.0511, 0.1383
R_1, wR_2 indices (all)	0.0296, 0.0760	0.0371, 0.0609	0.0599, 0.1463
GOF on F^2	1.341	0.948	1.108
	4	**5**	**6**
Formula	$H(H_3O)(C_6H_8N_2)(PbI_6)$	$(C_{36}H_{82}N_{10})(Pb_7I_{24})$	$(C_{40}H_{52}N_4)(Pb_4I_{12})\cdot H_2O$
Color and habit	colourless block	yellow rod	yellow rod
Crystal size (mm)	0.10 × 0.10 × 0.10	0.20 × 0.05 × 0.05	0.20 × 0.10 × 0.10

Crystal system	Hexagonal	Orthorhombic	Monoclinic
Space group	$P6_3mc$	$P2_12_12$	$P2_1/n$
a (Å)	10.1927(4)	15.5866(6)	9.1225(11)
b (Å)	10.1927(4)	32.6596(15)	22.378(3)
c (Å)	14.8276(10)	9.4273(4)	15.398(2)
α (°)	90	90	90
β (°)	90	90	95.343(2)
γ (°)	120	90	90
V (Å^3)	1334.07(12)	4799.0(4)	3129.9(7)
Z	2	2	2
Formula weight	1102.81	5151.05	2958.43
ρ_{calcd} (g cm^{-3})	2.745	3.565	3.139
μ (mm^{-1})	13.257	19.983	16.676
F(000)	952	4428	2588
θ (°)	4.73–25.48	3.14–25.50	2.42–25.50
Completeness	0.967	0.995	0.992
Index ranges of measured data	$-12 \le h \le 12$, $-12 \le k \le 12$, $-17 \le l \le 17$,	$-18 \le h \le 18$, $-39 \le k \le 39$, $-11 \le l \le 11$,	$-11 \le h \le 11$, $-27 \le k \le 25$, $-18 \le l \le 18$,
Reflections measured	8311	32319	23249
Indep. reflections (R_{int})	940 (0.0303)	8896 (0.0456)	5775 (0.0409)
Obs. reflections [$I > 2\sigma(I)$]	930	8042	4863
R_1, wR_2	0.0294, 0.0791	0.0277, 0.0425	0.0219, 0.0439

indices (obs.)			
R_1, wR_2	0.0297, 0.0792	0.0323, 0.0442	0.0257, 0.0448
indices (all)			
GOF on F^2	1.166	0.886	0.951

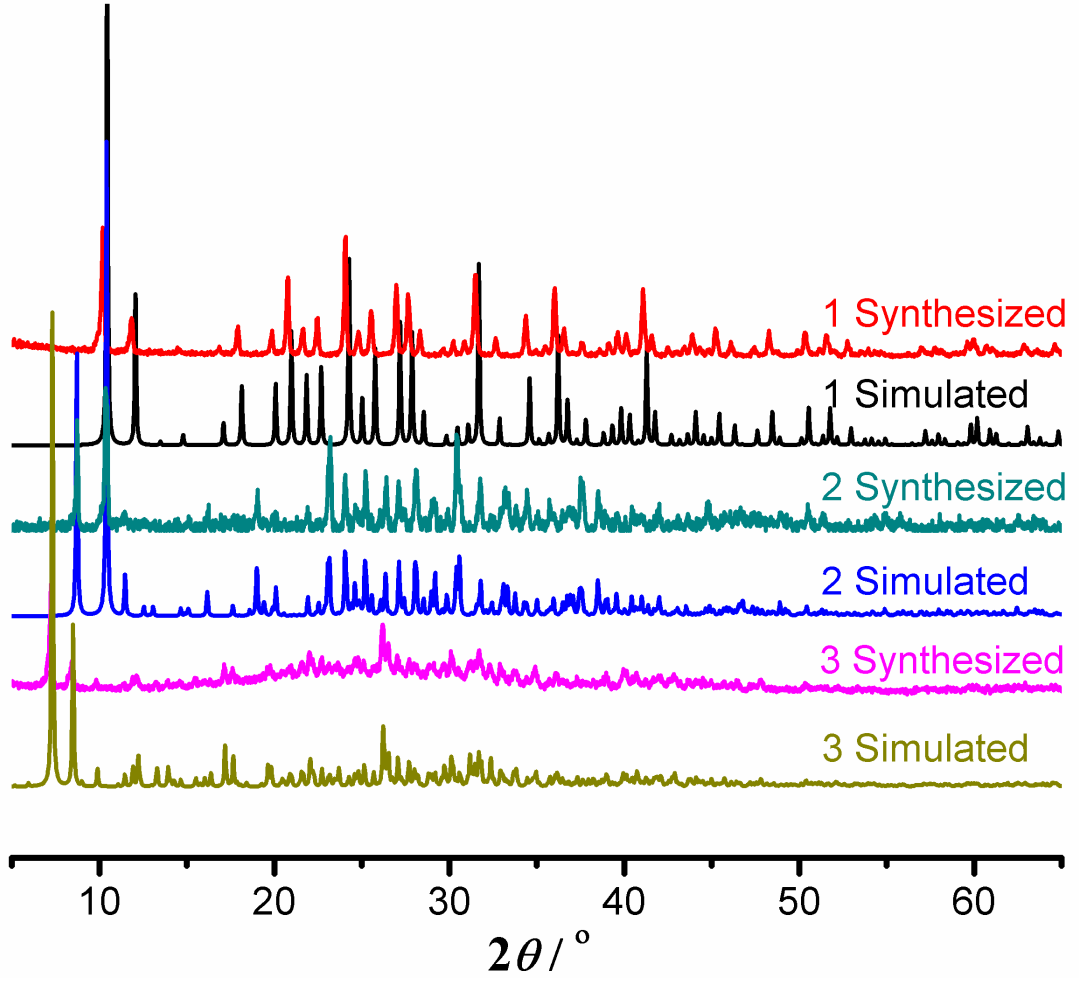

Fig. S1. PXRD patterns of **1**−**3**.

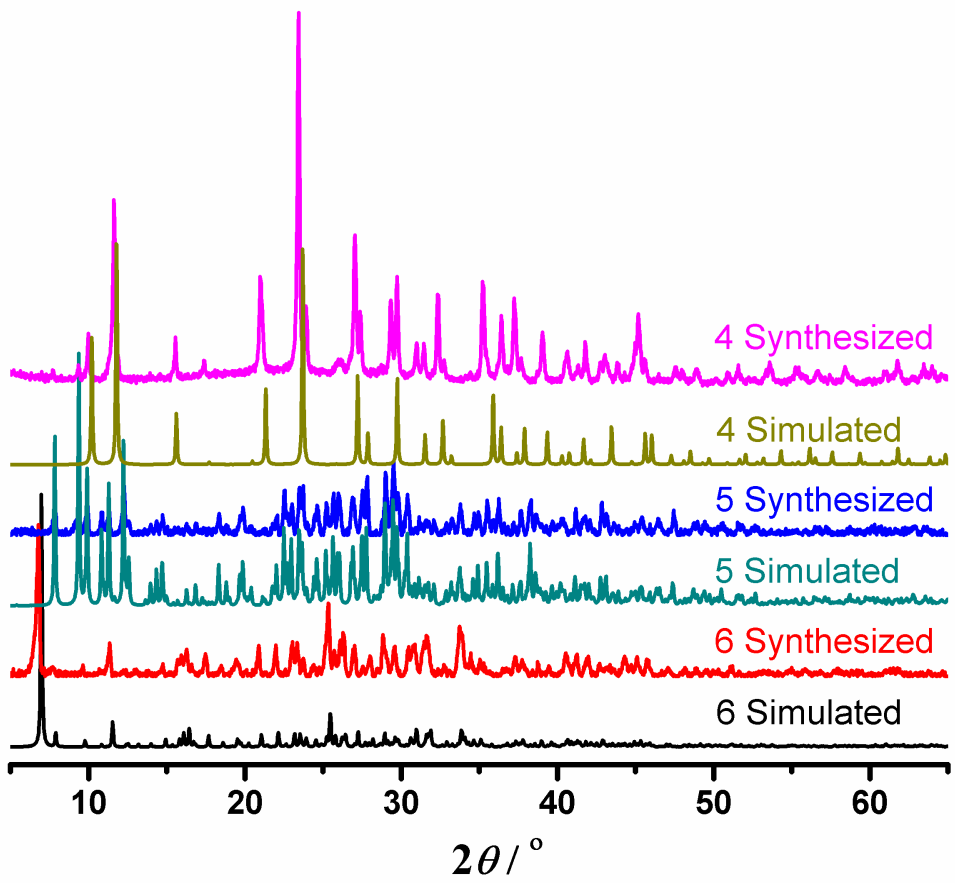

Figure S2. PXRD patterns of **4**−**6**.

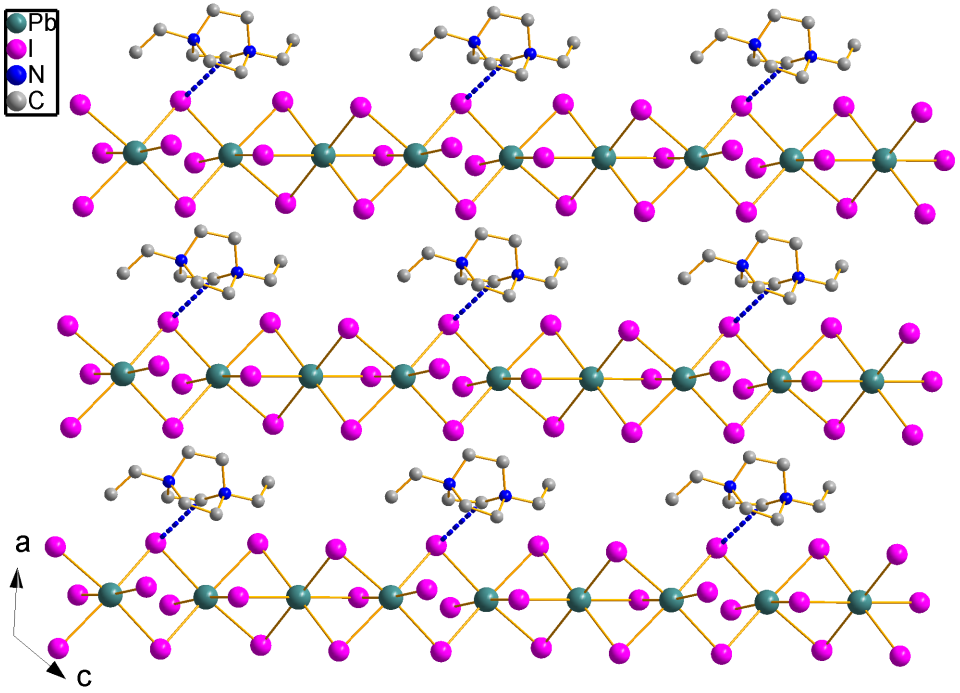

Fig. S3. Hydrogen-bonding scheme of **2**. Hydrogen atoms are omitted for clarity. The blue dashed lines represent the C−H···I hydrogen bonds.

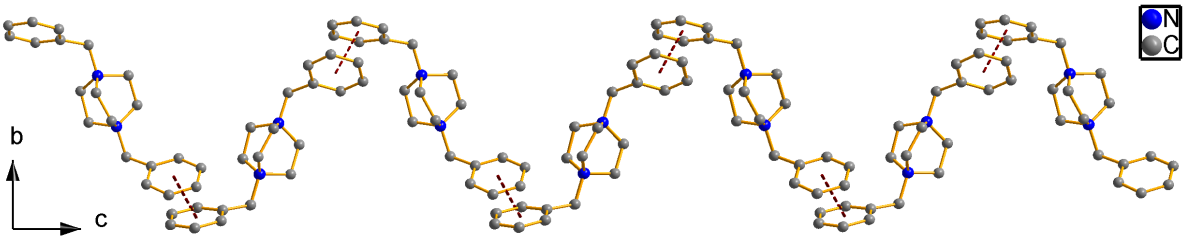

Fig. S4. $\pi\cdots\pi$ stacking interactions between two neighboring benzyl groups in **6**. Hydrogen atoms are omitted for clarity. The dashed lines represent the π···π interactions.