

Supporting Information

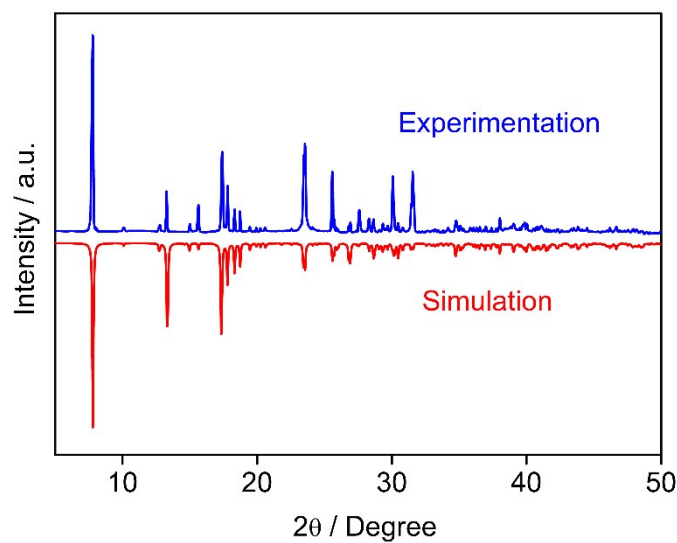


Figure S1. PXRD pattern of **1** measured at room temperature.

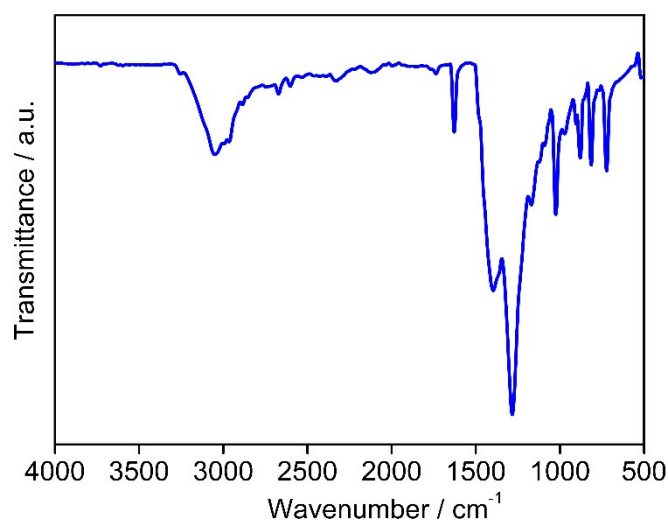


Figure S2. IR spectra of **1** measured at room temperature.

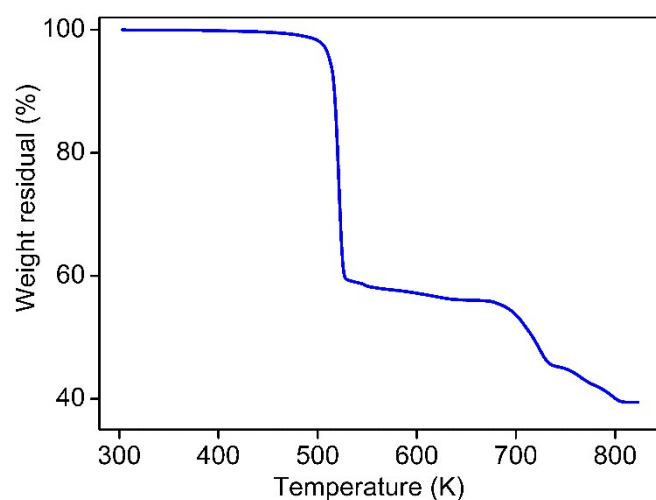


Figure S3. TGA curves of **1**.

Table S1. Bonds lengths (Å) and angles (°) for **1**.

1 (293 K)

Pb–O1	2.545(3)	O1–Pb–O2	44.74(9)
Pb–O2	2.929(4)	O1–Pb–O4	79.01(11)
Pb–O4	2.641(3)	O1–Pb–O5	76.95(12)
Pb–O5	2.608(3)	O1–Pb–O6 ⁱ	104.21(12)
Pb–O6 ⁱ	2.857(3)	O1–Pb–O7	141.14(10)
Pb–O7	2.710(4)	O1–Pb–O8	147.82(12)
Pb–O8	2.681(3)	O1–Pb–O10	66.83(9)
Pb–O10	2.691(3)	O1–Pb–O11 ⁱⁱ	107.69(10)
Pb–O11 ⁱⁱ	2.897(3)	O1–Pb–O12	86.22(10)
Pb–O12	2.756(3)	O2–Pb–O4	107.87(10)
		O2–Pb–O5	74.44(11)
		O2–Pb–O6 ⁱ	74.75(11)
		O2–Pb–O7	170.50(11)
		O2–Pb–O8	135.03(10)
		O2–Pb–O10	110.03(10)
		O2–Pb–O12	108.03(10)
		O4–Pb–O5	47.75(8)
		O4–Pb–O6 ⁱ	176.78(11)
		O4–Pb–O7	81.60(10)
		O4–Pb–O8	71.41(11)
		O4–Pb–O10	63.98(9)
		O4–Pb–O11 ⁱⁱ	113.78(9)
		O4–Pb–O12	108.55(9)
		O5–Pb–O6 ⁱ	132.52(9)
		O5–Pb–O7	112.81(10)
		O5–Pb–O8	73.91(11)
		O5–Pb–O10	106.91(9)

O5–Pb–O11 ⁱⁱ	69.18(9)
O5–Pb–O12	152.88(9)
O6 ⁱ –Pb–O7	95.76(11)
O6 ⁱ –Pb–O8	105.43(12)
O6 ⁱ –Pb–O10	117.18(10)
O6 ⁱ –Pb–O11 ⁱⁱ	65.37(9)
O6 ⁱ –Pb–O12	71.99(9)
O7–Pb–O8	46.41(9)
O7–Pb–O10	74.43(10)
O7–Pb–O11 ⁱⁱ	110.90(11)
O7–Pb–O12	68.58(9)
O8–Pb–O10	109.23(10)
O8–Pb–O11 ⁱⁱ	74.22(9)
O8–Pb–O12	114.75(9)
O10–Pb–O11 ⁱⁱ	174.19(9)
O10–Pb–O12	46.25(9)
O11 ⁱⁱ –Pb–O12	137.15(9)

Symmetry codes: (i) 1+x, y, z; (ii) x, 3/2–y, 1/2+z.

1 (373 K)

Pb–O3 ⁱ	2.60(2)	O3–Pb–O3 ⁱ	33.9(12)
Pb–O3 ⁱⁱ	2.60(2)	O3–Pb–O3 ⁱⁱ	33.9(12)
Pb–O3 ⁱⁱⁱ	2.60(2)	O3–Pb–O3 ⁱⁱⁱ	33.9(12)
Pb–O3 ^{iv}	2.60(2)	O3–Pb–O3 ^{iv}	33.9(12)
Pb–O3 ^{vi}	2.60(2)	O3–Pb–O3 ^v	48.6(18)
Pb–O3 ^{vii}	2.60(2)	O3–Pb–O3 ^{vi}	146.1(12)
Pb–O3 ^{viii}	2.60(2)	O3–Pb–O3 ^{vii}	131.4(18)
Pb–O3 ^x	2.60(2)	O3–Pb–O3 ^{viii}	146.1(12)
Pb–O3 ^{xi}	2.60(2)	O3–Pb–O3 ^{ix}	180.0
Pb–O3_1	2.63(3)	O3 ⁱ –Pb–O3 ⁱⁱ	0.0(17)
Pb–O3 ⁱ _1 ^{xii}	2.63(3)	O3 ⁱ –Pb–O3 ⁱⁱⁱ	48.6(18)
Pb ^{xv} –O1_1	2.72(3)	O3 ⁱ –Pb–O3 ^{iv}	48.6(18)
		O3 ⁱ –Pb–O3 ^v	33.9(12)
		O3 ⁱ –Pb–O3 ^{vi}	131.4(18)
		O3 ⁱ –Pb–O3 ^{vii}	146.1(12)
		O3 ⁱ –Pb–O3 ^{viii}	180.0
		O3 ⁱ –Pb–O3 ^{ix}	146.1(12)
		O3 ⁱⁱ –Pb–O3 ⁱⁱⁱ	48.6(18)
		O3 ⁱⁱ –Pb–O3 ^{iv}	48.6(18)
		O3 ⁱⁱ –Pb–O3 ^v	33.9(12)
		O3 ⁱⁱ –Pb–O3 ^{vi}	131.4(18)
		O3 ⁱⁱ –Pb–O3 ^{vii}	146.1(12)
		O3 ⁱⁱ –Pb–O3 ^{viii}	180.0
		O3 ⁱⁱ –Pb–O3 ^{ix}	146.1(12)

O3 ⁱⁱⁱ —Pb—O3 ^{iv}	0.0(18)
O3 ⁱⁱⁱ —Pb—O3 ^v	33.9(12)
O3 ⁱⁱⁱ —Pb—O3 ^{vi}	180.0
O3 ⁱⁱⁱ —Pb—O3 ^{vii}	146.1(12)
O3 ⁱⁱⁱ —Pb—O3 ^{viii}	131.4(18)
O3 ⁱⁱⁱ —Pb—O3 ^{ix}	146.1(12)
O3 ^{iv} —Pb—O3 ^v	33.9(12)
O3 ^{iv} —Pb—O3 ^{vi}	180.0
O3 ^{iv} —Pb—O3 ^{vii}	146.1(12)
O3 ^{iv} —Pb—O3 ^{viii}	131.4(18)
O3 ^{iv} —Pb—O3 ^{ix}	146.1(12)
O3 ^v —Pb—O3 ^{vi}	146.1(12)
O3 ^v —Pb—O3 ^{vii}	180.0
O3 ^v —Pb—O3 ^{viii}	146.1(12)
O3 ^v —Pb—O3 ^{ix}	131.4(18)
O3 ^{vi} —Pb—O3 ^{vii}	33.9(12)
O3 ^{vi} —Pb—O3 ^{viii}	48.6(18)
O3 ^{vi} —Pb—O3 ^{ix}	33.9(12)
O3 ^{vii} —Pb—O3 ^{viii}	33.9(12)
O3 ^{vii} —Pb—O3 ^{ix}	48.6(18)
O3 ^{viii} —Pb—O3 ^{ix}	33.9(12)
O3_1—Pb—O3	132.3(10)
O3_1—Pb—O3 ⁱ	106.4(5)
O3_1—Pb—O3 ⁱⁱ	106.4(5)
O3_1—Pb—O3 ⁱⁱⁱ	106.4(5)
O3_1—Pb—O3 ^{iv}	106.4(5)
O3_1—Pb—O3 ^v	83.7(11)
O3_1—Pb—O3 ^{vi}	73.6(5)
O3_1—Pb—O3 ^{vii}	96.3(11)
O3_1—Pb—O3 ^{viii}	73.6(5)
O3_1—Pb—O3 ^{ix}	47.7(10)
O3_1—Pb—O3 ^x	36.0(10)
O3_1 ^x —Pb—O3	96.3(11)
O3_1 ^x —Pb—O3 ⁱ	73.6(5)
O3_1 ^x —Pb—O3 ⁱⁱ	73.6(5)
O3_1 ^x —Pb—O3 ⁱⁱⁱ	73.6(5)
O3_1 ^x —Pb—O3 ^{iv}	73.6(5)
O3_1 ^x —Pb—O3 ^v	47.7(10)
O3_1 ^x —Pb—O3 ^{vi}	106.4(5)
O3_1 ^x —Pb—O3 ^{vii}	132.3(10)
O3_1 ^x —Pb—O3 ^{viii}	106.4(5)
O3_1 ^x —Pb—O3 ^{ix}	83.7(11)

Symmetry codes: (i) 1+y, -1+x, z; (ii) 1+y, -x, z; (iii) -y, -x, z; (iv) -y, -1+x, z; (v) 1-x, -1-y, Z; (vi) 1+y, -x, 1-z; (vii) x, y, 1-z; (viii) -y, -1+x, 1-z; (ix) 1-x, -1-y,

$1-z$; (x) $1-x$, y , $1-z$; (xv) x , $1+y$, z .

Table S2. Selected hydrogen bonds (Å, °) for **1**.

D–H···A	H···A	D···A	D–H···A
1 (293 K)			
N5–H5A···O1	1.97	2.806(5)	156.7
N5–H5A···O3	2.57	3.364(6)	149.8
N5–H5B···O8 ⁱ	2.01	2.884(5)	167.3
N5–H5B···O9 ⁱ	2.51	3.222(5)	137.4
N6–H6A···O5	2.02	2.903(4)	171.4
N6–H6A···O6	2.64	3.230(5)	124.8
N6–H6B···O11 ⁱⁱⁱ	2.51	3.159(5)	129.9
N6–H6B···O12 ⁱⁱⁱ	2.13	3.019(4)	175.9
Symmetry codes: (i) x , $3/2-y$, $-1/2+z$; (ii) $1-x$, $-1/2+y$, $1/2-z$; (iii) $-1+x$, $3/2-y$, $1/2+z$.			