Supporting Information

Synthesis, Physico-Chemical Characterization and Structure of the Elusive Hydroxylammonium Lead Iodide Perovskite NH_3OHPbI_3

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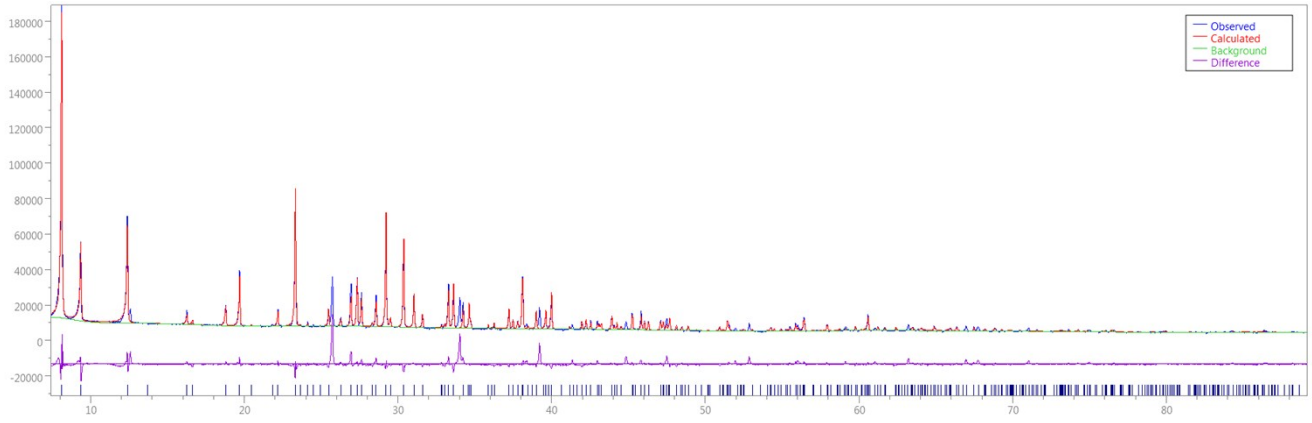

Fig. S1. Le Bail fit of the X-ray powder diffraction pattern of NH_3OHPbI_3 powder prepared by sulfolane extraction with toluene. The peaks that were not fitted are attributed to PbI_2 impurity.

Bond lengths

Pb1—I2	3.2060 (7)	C1—H1AB	0.9900
Pb1—I2^{i}	3.2060 (7)	C1—H1AA	0.9900
Pb1—I3	3.2160 (5)	C1—C2AB	1.53 (2)
Pb1—I3^{i}	3.2159 (5)	C1—C2AA	1.53 (2)
Pb1—I3^{ii}	3.2159 (5)	C2AB—H2AA	0.9900
Pb1—I3^{iii}	3.2159 (5)	C2AB—H2AB	0.9900
S4—O3	1.33 (2)	C2AA—H2AC	0.9900
S4—O3^{iv}	1.33 (2)	C2AA—H2AD	0.9900
S4—C2AB	1.878 (15)	O2—H2	0.8401
S4—C2AA	1.881 (15)	O2—N3	1.4151 (10)
C1—C1^{iv}	1.52 (2)	N3—H3A	0.9099
C1—H1BD	0.9900	N3—H3B	0.9100
C1—H1BC	0.9900	N3—H3C	0.9101
Bond angles			
I2—Pb1—I2^{i}	180.0	C1^{iv}—C1—C2AA	118.0 (8)
I2^{i}—Pb1—I3^{iii}	93.005 (13)	H1BD—C1—H1BC	108.0
I2^{i}—Pb1—I3^{i}	86.995 (13)	H1AB—C1—H1AA	107.1
I2—Pb1—I3^{ii}	93.005 (13)	C2AB—C1—H1BD	109.4
I2—Pb1—I3^{i}	93.005 (13)	C2AB—C1—H1BC	109.4
I2^{i}—Pb1—I3^{ii}	86.995 (13)	C2AA—C1—H1AB	107.8
I2—Pb1—I3	86.995 (13)	C2AA—C1—H1AA	107.8
I2—Pb1—I3^{iii}	86.995 (13)	S4—C2AB—H2AA	112.1
I2^{i}—Pb1—I3	93.005 (13)	S4—C2AB—H2AB	112.1
I3^{iii}—Pb1—I3^{i}	96.06 (2)	C1—C2AB—S4	98.3 (10)
I3^{i}—Pb1—I3	180.0	C1—C2AB—H2AA	112.1
I3^{iii}—Pb1—I3	83.94 (2)	C1—C2AB—H2AB	112.1
I3^{ii}—Pb1—I3^{iii}	180.00 (2)	H2AA—C2AB—H2AB	109.8
I3^{ii}—Pb1—I3^{i}	83.94 (2)	S4—C2AA—H2AC	112.1
I3^{ii}—Pb1—I3	96.06 (2)	S4—C2AA—H2AD	112.1
Pb1^{iii}—I2—Pb1	76.281 (19)	C1—C2AA—S4	98.1 (10)
Pb1^{iii}—I3—Pb1	76.003 (14)	C1—C2AA—H2AC	112.1
O3—S4—O3^{iv}	102 (3)	C1—C2AA—H2AD	112.1
O3—S4—C2AB	130.9 (12)	H2AC—C2AA—H2AD	109.8
O3^{iv}—S4—C2AB	98.3 (12)	N3—O2—H2	107.4
O3—S4—C2AA	107.1 (12)	O2—N3—H3A	104.9

O3^{iv}—S4—C2AA	118.1 (12)	O2—N3—H3B	102.7
C1^{iv}—C1—H1BD	109.4	O2—N3—H3C	120.3
C1^{iv}—C1—H1BC	109.4	H3A—N3—H3B	109.5
C1^{iv}—C1—H1AB	107.8	H3A—N3—H3C	109.5
C1^{iv}—C1—H1AA	107.8	H3B—N3—H3C	109.4
C1^{iv}—C1—C2AB	111.3 (10)		
C1^{iv}—C1—C2AB—S4	−35.2 (18)	O3^{iv}—S4—C2AB—C1	147.1 (17)
C1^{iv}—C1—C2AA—S4	12 (2)	O3—S4—C2AA—C1	−130.7 (18)
O3—S4—C2AB—C1	−100 (2)	O3^{iv}—S4—C2AA—C1	115.5 (18)

Table S1. Geometrical parameters (bond lengths and angles) of the structure. Bond lengths and angles are reported in Ångstroms and degrees, respectively.