Supporting information

Structure and Function Relationships in Alkylammonium Lead(II) iodide Solar Cells

Majid Safdari[a], Andreas Fischer[a], Bo Xu[b], Lars Kloo[a] and James Gardner[a*]

[a] Division of Applied Physical Chemistry, Department of Chemistry, KTH Royal Institute of Technology, SE-100 44, Stockholm, Sweden.
[b] Organic Chemistry, Center of Molecular Devices, Department of Chemistry, KTH Chemical Science and Engineering, 10044, Stockholm, Sweden

Table S1 Atomic parameters for $PAPbI_3$ obtained from single crystallography characterization.

Atom	Ox.	Wyck.	Site	x/a	y/b	z/c	U [Å2]
C1		4a	1	0.2273(7)	0.1452(8)	0.2727(14)	
C2		4a	1	0.2468(11)	0.1636(13)	0.4591(18)	
H2A		4a	1	0.29020	0.11240	0.54210	0.0790
H2B		4a	1	0.19610	0.15770	0.47960	0.0790
C3		4a	1	0.2832(7)	0.2886(11)	0.4914(14)	
H3A		4a	1	0.24210	0.34100	0.49590	0.0560
H3B		4a	1	0.33750	0.29550	0.60460	0.0560
C4		4a	1	0.2936(9)	0.2999(12)	0.313(2)	
H4A		4a	1	0.27270	0.37120	0.25530	0.0800
H4B		4a	1	0.35380	0.29350	0.34210	0.0800
C5		4a	1	0.0521(5)	0.1365(7)	0.6794(13)	
H5A		4a	1	0.03980	0.13930	0.54700	0.0390
H5B		4a	1	0.03210	0.20460	0.71020	0.0390
C6		4a	1	0.0073(10)	0.0424(11)	0.7116(19)	
H6A		4a	1	0.01040	0.04600	0.83710	0.0760
H6B		4a	1	0.03250	-0.02660	0.69940	0.0760
C7		4a	1	-0.0877(8)	0.0519(11)	0.556(3)	
H7A		4a	1	-0.09210	0.10900	0.46860	0.1230
H7B		4a	1	-0.12410	0.06940	0.61490	0.1230
H7C		4a	1	-0.10560	-0.01700	0.49030	0.1230
I1		4a	1	-0.11127(3)	0.60408(5)	0.00770(5)	
I2		4a	1	0.02638(6)	0.29529(3)	0.14575(16)	
I3		4a	1	0.16674(2)	0.41053(4)	0.78304(5)	
N1		4a	1	0.1443(5)	0.1254(7)	0.7969(18)	
H1A		4a	1	0.16920	0.19140	0.81390	0.0870
H1B		4a	1	0.16620	0.08070	0.74010	0.0870
H1C		4a	1	0.15420	0.09710	0.90900	0.0870
O1		4a	1	0.2495(5)	0.2218(7)	0.2000(11)	
O2		4a	1	0.1860(6)	0.0651(7)	0.1792(11)	
Pb1		4a	1	0.02364(4)	0.49982(3)	0.39451(10)	

Table S2: Atomic parameters for $MAPbI_3$ obtained from single crystallography characterization.

Atom	Ox.	Wyck.	Site	S.O.F.	x/a	y/b	z/c	U [Å2]
Pb1		1a	m-3m		0	0	0	
I2		3d	4/mm.m		1/2	0	0	

Table S3 Bond length and angles in the $MAPbI_3$, $EAPbI_3$ and $PAPbI_3$

	MAPbI3	EAPbI327	PAPbI3
Angle Pb-I-Pb-1	180°	74.19°	77.04°
Angle Pb-I-Pb-2		72.16°	77.23°
Angle Pb-I-Pb-3		72.16°	77.85°
Angle Pb-I-Pb-4		85.9°	
Angle Pb-I-Pb-5		85.9°	
Angle Pb-I-Pb-6		84.02°	
Angle Pb-I-Pb-7		73.9°	
Angle Pb-I-Pb-8		73.9°	
Angle Pb-I-Pb-9		72.92°	
Angle Pb-I-Pb-10		81.5°	
Angle Pb-I-Pb-11		81.5°	
Angle Pb-I-Pb-12		75.27°	
Angle I-Pb-I-1	180°	172.74°	175.88°
Angle I-Pb-I-2		178.83°	176.12°
Angle I-Pb-I-3		172.74°	178.42°
Angle I-Pb-I-4		172.02°	
Angle I-Pb-I-5		175.08°	
Angle I-Pb-I-6		172.02°	
Bond length Pb-I-1	3.14 Å	3.025 Å	3.195 Å
Bond length Pb-I-2		3.098 Å	3.215 Å
Bond length Pb-I-3		3.098 Å	3.225 Å
Bond length Pb-I-4		3.302 Å	3.234 Å
Bond length Pb-I-5		3.302 Å	3.245 Å
Bond length Pb-I-6		3.361 Å	3.251 Å
Bond length Pb-I-7		3.294 Å	
Bond length Pb-I-8		3.294 Å	
Bond length Pb-I-9		3.331 Å	
Bond length Pb-I-10		3.208 Å	
Bond length Pb-I-11		3.208 Å	
Bond length Pb-I-12		3.429 Å	

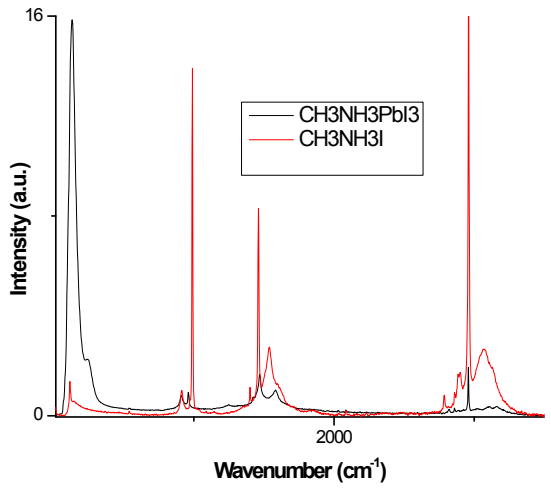

Figure S1. Raman spectra of CH_3NH_3I and $CH_3NH_3PbI_3$

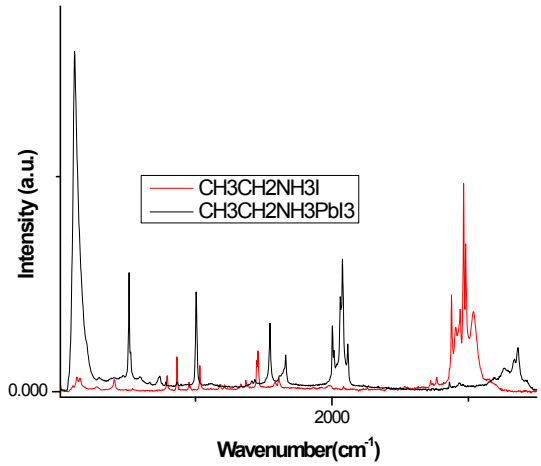

Figure S2. Raman spectra of $CH_3CH_2NH_3I$ and $CH_3CH_2NH_3PbI_3$

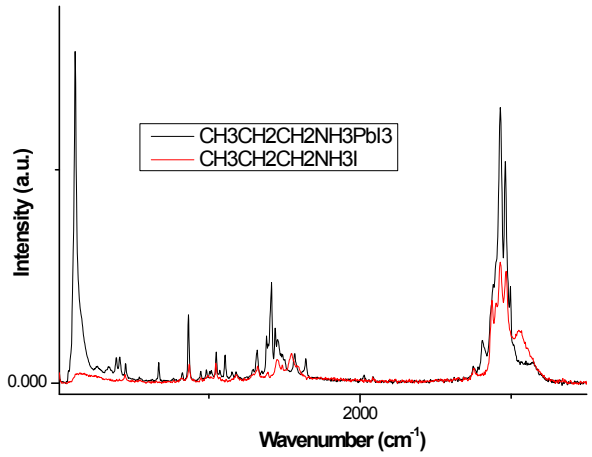

Figure S3. Raman spectra of $CH_3CH_2CH_2NH_3I$ and $CH_3CH_2CH_2NH_3PbI_3$