Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Novel design strategies for perovskite materials with improved stability and suitable band gaps

Bing Zhang,*[a,b] Xiaogang Wang,[b] ,Yang Yang,[b] Bin Hu,[a,b] Lei Tong,[b] Li Zhao,[a,b] Qiang Lu[a,b]

[a.] National Engineering Laboratory for Biomass Power Generation Equipment, North China Electric Power University, Beijing 102206, P. R. China.

[b.] School of New Energy, North China Electric Power University, Beijing 102206, P. R. China;

[*] Corresponds author: Email: 51101869@ncepu.edu.cn ; Tel: +86-10-61772079. Fax: +86-10-61772079

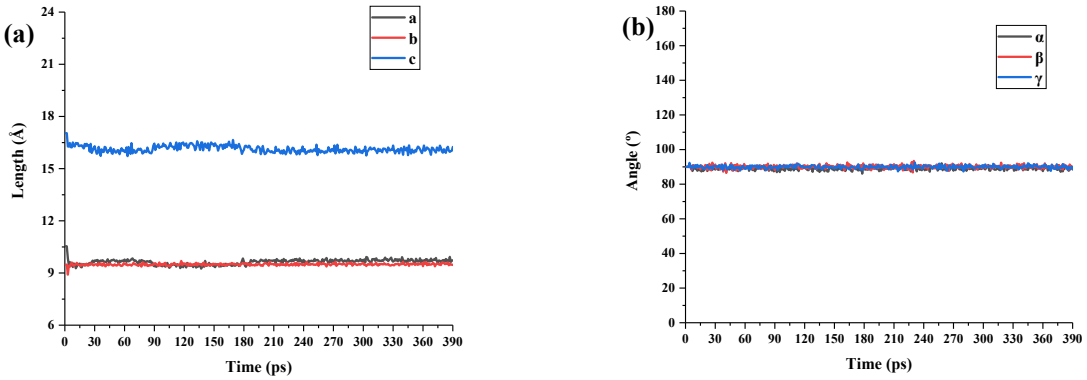

Fig. S1 The lattice parameters of a, b, c (a) and α, β, γ (b) of the NH_4PbI_3 system.

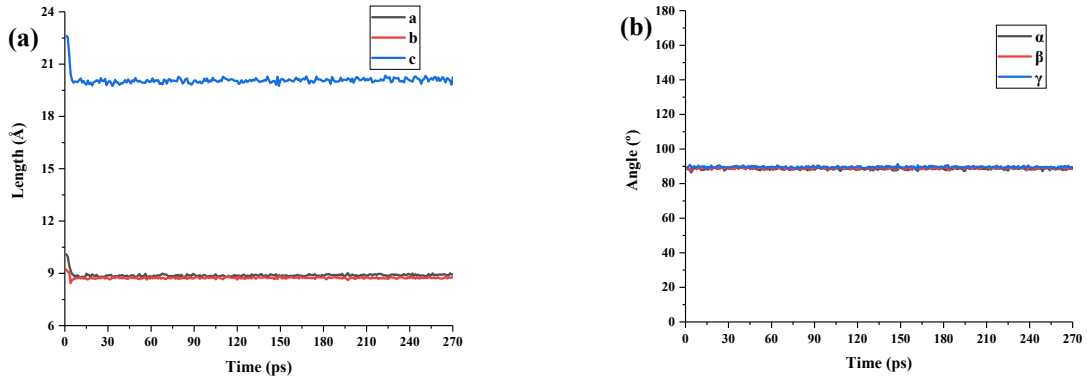

Fig. S2 The lattice parameters of a, b, c (a) and α, β, γ (b) of the $NH_4PbI_3 \bullet 2H_2O$ system.

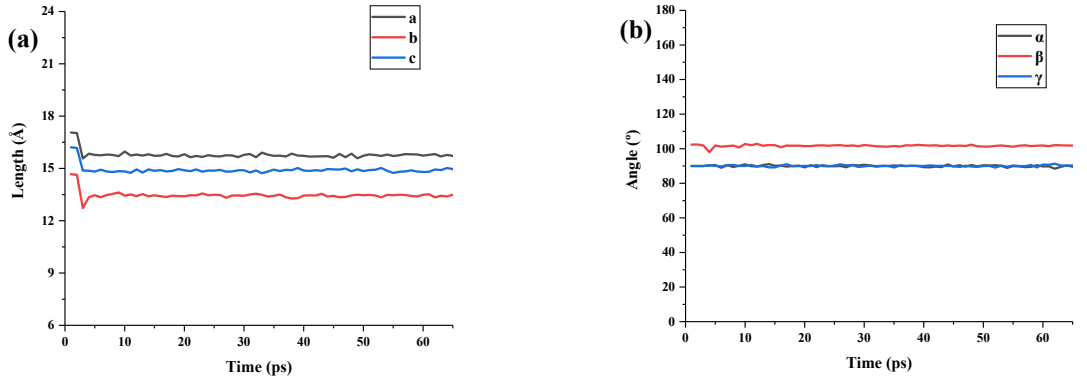

Fig. S3 The lattice parameters of a, b, c (a) and α, β, γ (b) of the $Ni(C_{10}H_8N_2)_3Pb_2I_6$ system.

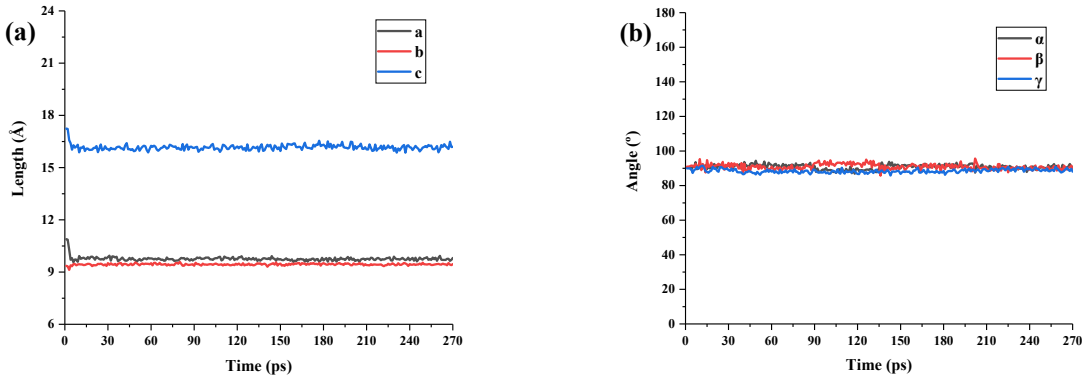

Fig. S4 The lattice parameters of a, b, c (a) and α, β, γ (b) of the $(NH_4)_{0.875}(GUA)_{0.125}PbI_3$ system.

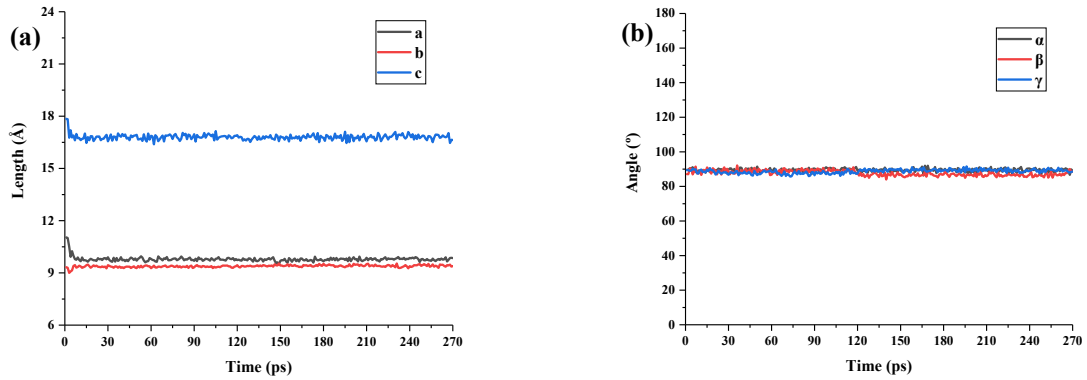

Fig. S5 The lattice parameters of a, b, c (a) and α, β, γ (b) of the $(NH_4)_{0.750}(GUA)_{0.250}PbI_3$ system.

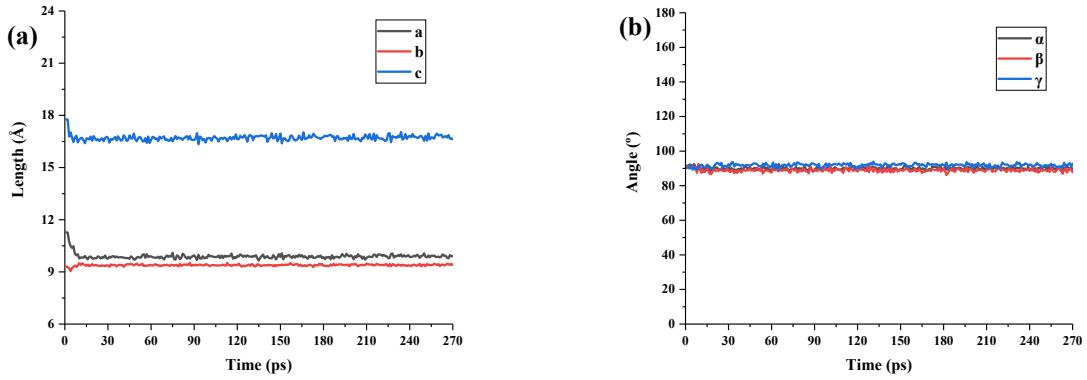

Fig. S6 The lattice parameters of a, b, c (a) and α, β, γ (b) of the $(NH_4)_{0.625}(GUA)_{0.375}PbI_3$ system.

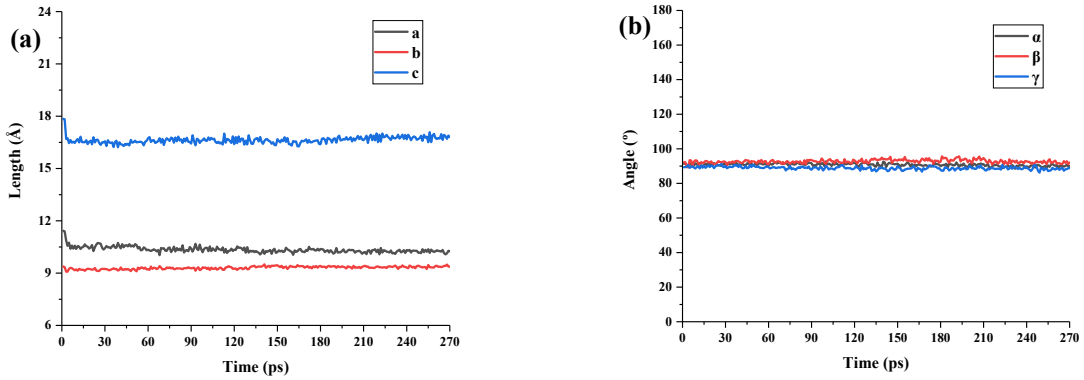

Fig. S7 The lattice parameters of a, b, c (a) and α, β, γ (b) of the $(NH_4)_{0.500}(GUA)_{0.500}PbI_3$ system.

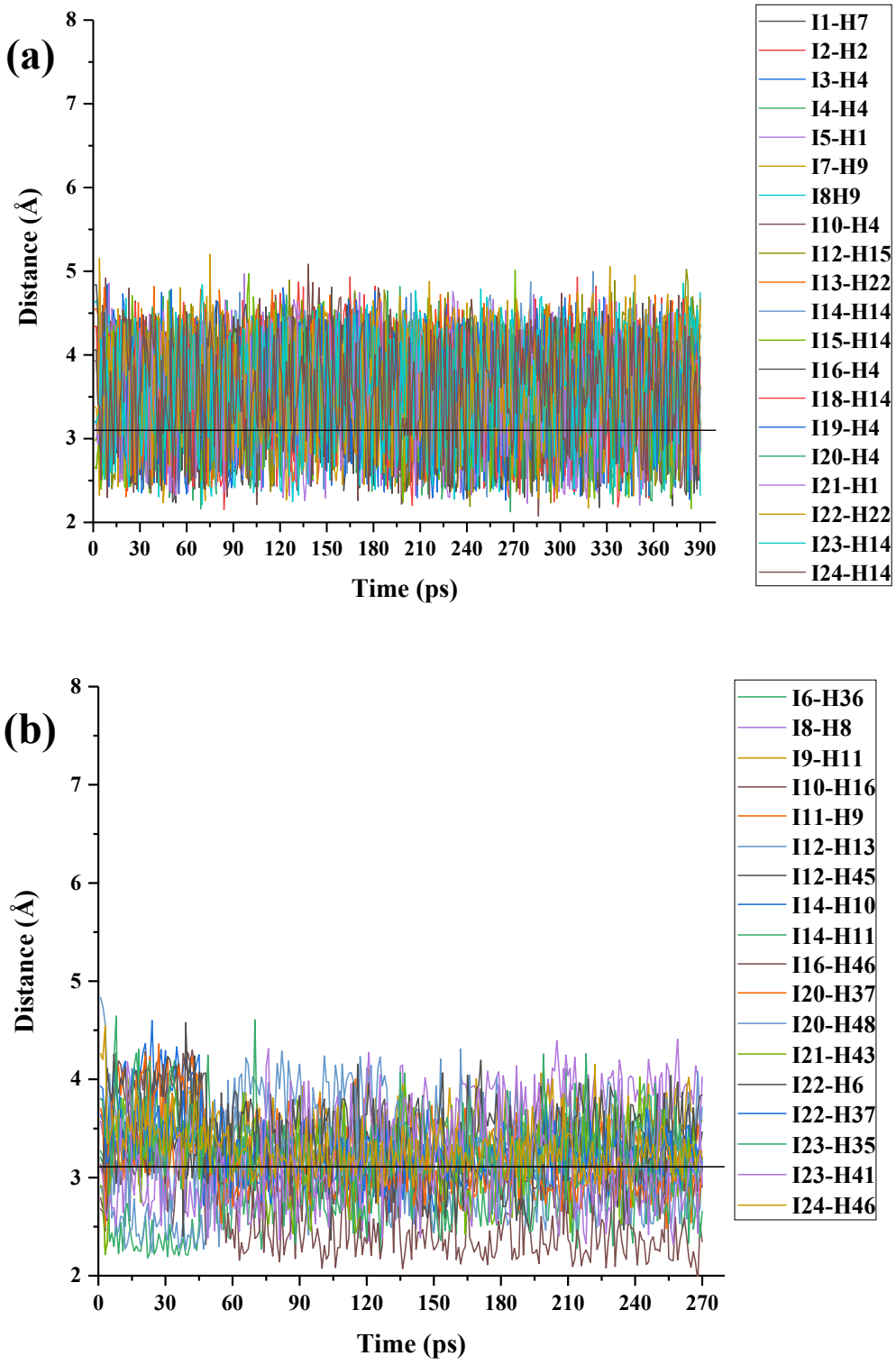

Fig. S8 Typical (a) N-H…I HBs in NH_4PbI_3, and (b) O-H…I HBs in $NH_4PbI_3 \bullet 2H_2O$, respectively. The black horizontal lines represent the normal bond length H…I in N-H…I HBs of 3.10 Å and in O-H…I HBs of 3.11 Å.

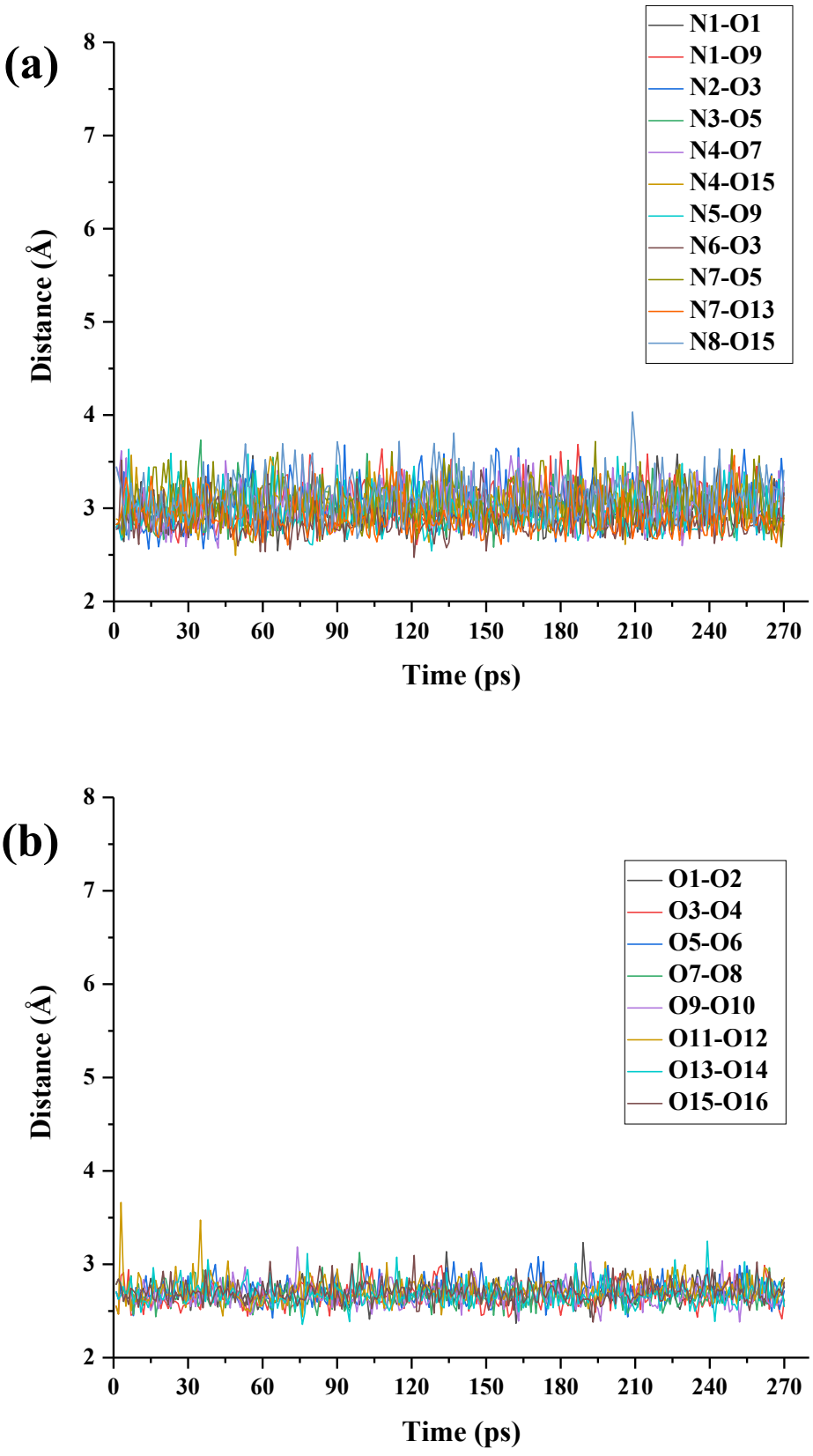

Fig. S9 The distance of (a) N-O, and (b) O-O of the HB networks in $NH_4PbI_3 \bullet 2H_2O$ system.

In this work, all the average distances of I-H less than 4.00 Å were counted as seen in Table S1.

Table S1 The average distances of I-H less than 4.00 Å in $(NH_4)_{1-x}(GUA)_xPbI_3$(x = 0.125, 0.250, 0.375, 0.500) and NH_4PbI_3 system.

x = 0.125		x = 0.250		x = 0.375		x = 0.500		NH_4PbI_3	
I-H	Distance (Å)	I-H	Distance (Å)	I-H	Distance(Å)	I-H	Distance (Å)	I-H	Distance (Å)
I1-H32	3.62	I1-H6	3.69	I1-H36	2.6	I1-H20	3.22	I1-H7	3.50
I1-H34	3.69	I1-H29	2.63	I2-H21	2.92	I1-H36	2.53	I2-H2	3.61
I2-H25	3.53	I1-H30	3.69	I3-H2	3.5	I1-H37	2.77	I3-H4	3.55
I3-H28	3.56	I3-H2	3.69	I3-H24	2.96	I2-H14	3.01	I4-H4	3.63
I4-H1	3.72	I3-H3	3.74	I3-H26	2.35	I3-H1	3.47	I5-H1	3.59
I4-H3	3.47	I4-H7	3.14	I4-H18	3.57	I3-H17	2.62	I7-H9	3.57
I4-H6	3.42	I4-H9	3.61	I4-H32	2.55	I3-H28	3.04	I8-H9	3.62
I4-H19	3.49	I4-H18	3.56	I4-H34	2.5	I4-H39	2.53	I10-H4	3.60
I9-H7	3.63	I4-H28	2.80	I4-H35	2.78	I4-H8	3.58	I12-H15	3.58
I9-H8	3.50	I5-H24	3.50	I4-H7	3.6	I5-H22	3.23	I13-H22	3.65
I9-H27	3.75	I5-H31	3.55	I5-H30	2.95	I7-H3	3.58	I14-H14	3.61
I10-H28	2.90	I6-H22	3.09	I5-H32	3.38	I8-H8	3.56	I15-H14	3.60
I13-H10	3.46	I6-H33	3.35	I6-H21	3.53	I9-H13	2.7	I16-H4	3.52
I13-H16	3.70	I6-H34	3.51	I6-H29	3.04	I9-H14	2.83	I18-H14	3.63
I13-H20	3.42	I6-H36	3.52	I9-H21	2.95	I9-H4	3.48	I19-H4	3.59
I14-H7	3.71	I7-H35	3.19	I10-H30	3	I13-H37	3.36	I20-H4	3.56
I14-H8	3.72	I11-H30	3.40	I11-H37	3.48	I14-H4	3.4	I21-H1	3.60
I16-H11	3.48	I12-H4	3.42	I11-H38	2.92	I10-H15	3.07	I22-H22	3.66
I16-H13	3.50	I13-H17	3.25	I12-H24	2.67	I13-H19	2.54	I23-H14	3.62
I21-H9	3.66	I14-H1	3.54	I13-H15	3.56	I13-H5	3.44	I24-H14	3.60
I21-H18	3.78	I14-H2	3.50	I13-H6	3.45	I14-H15	3.05	-	-
I22-H16	3.61	I14-H10	3.42	I14-H20	3.56	I14-H25	2.92	-	-
-	-	I14-H19	3.63	I14-H22	2.64	I14-H4	3.4	-	-
-	-	I14-H20	3.69	I14-H23	3.29	I15-H16	2.87	-	-
-	-	I15-H19	3.76	I14-H5	3.26	I15-H18	2.43	-	-
-	-	I16-H16	3.50	I15-H14	3.41	I15-H6	3.59	-	-
-	-	I19-H14	3.20	I16-H5	3.42	I16-H39	3.26	-	-
-	-	I21-H10	3.56	I17-H30	3.06	I16-H40	2.95	-	-
-	-	I23-H15	3.63	I17-H35	3.31	I17-H40	3.17	-	-

x = 0.125		x = 0.250		x = 0.375		x = 0.500		NH_4PbI_3	
I-H	Distance (Å)	I-H	Distance (Å)	I-H	Distance(Å)	I-H	Distance (Å)	I-H	Distance (Å)
-	-	-	-	I18-H28	3.51	I18-H36	2.76	-	-
-	-	-	-	I19-H11	3.53	I20-H5	3.54	-	-
-	-	-	-	I23-12	3.33	I21-H25	2.74	-	-
-	-	-	-	-	-	I22-H30	2.68	-	-
-	-	-	-	-	-	I22-H38	3.11	-	-
-	-	-	-	-	-	I22-H40	3.48	-	-