Electronic Supplementary Information

B-Site Substitution Effect on the Mechanical Properties of Halide Perovskites $[C_4H_{12}N_2][BCl_3]\cdot H_2O$ ($B = NH_4^+; K^+$)

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Table S1 Comparison of cell parameters of PIP-NH_4 and PIP-K.

Compound	$[C_4H_{12}N_2][NH_4Cl_3]\cdot H_2O$[#]	$[C_4H_{12}N_2][KCl_3]\cdot H_2O$
Formula	$C_4H_{18}Cl_3N_3O$	$C_4H_{14}Cl_3KN_2O$
M_w	230.56	251.62
T/K	120(10)	120(10)
Crystal system	orthorhombic	orthorhombic
Space group	Pbcm	Pbcm
a(Å)	6.4777(12)	6.4153(8)
b(Å)	12.8490(2)	12.7348(3)
c(Å)	12.7491(2)	12.7219(3)
V(Å^3)	1061.14(3)	1039.35(4)
Z	4	4
Radiation	-	Cu
2θ range for data collection (°)	-	13.804-146.174
$\rho_{calcd.}$/ (g·cm^{-3})	-	1.608
μ / mm^{-1}	-	11.214
F (000)	-	520.0
GOF	-	1.205
R_1[a] [I >2s(I)]	-	R_1=0.0381, wR_2=0.0960
wR_2[b](all data)	-	R_1=0.0384, wR_2=0.0963

a, $R_1 = \sum||F_o|-|F_c||/\sum|F_o|$; *b*, $wR_2 = [\sum w(F_o^2-F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$.

[#]Note: These data are referenced from the reported data.[1]

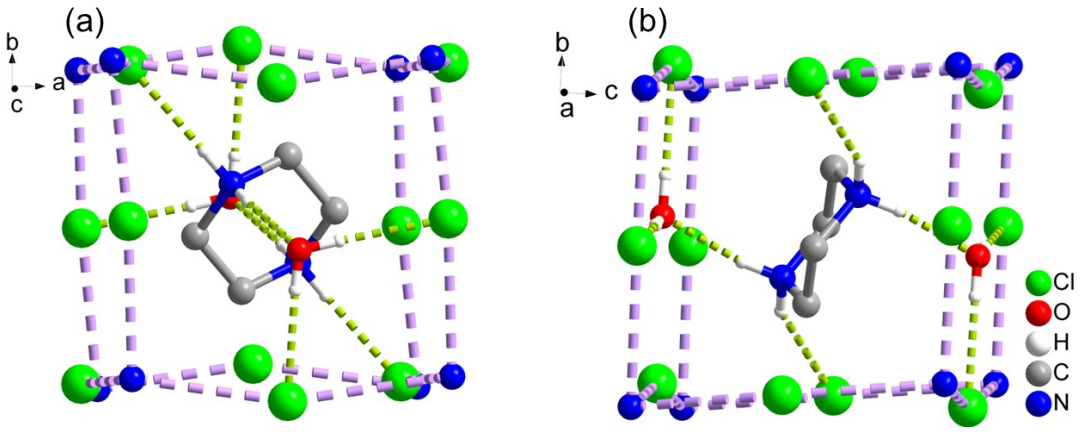

Figure S1. Hydrogen bond diagrams of $[C_4H_{12}N_2][NH_4Cl_3]\cdot H_2O$.

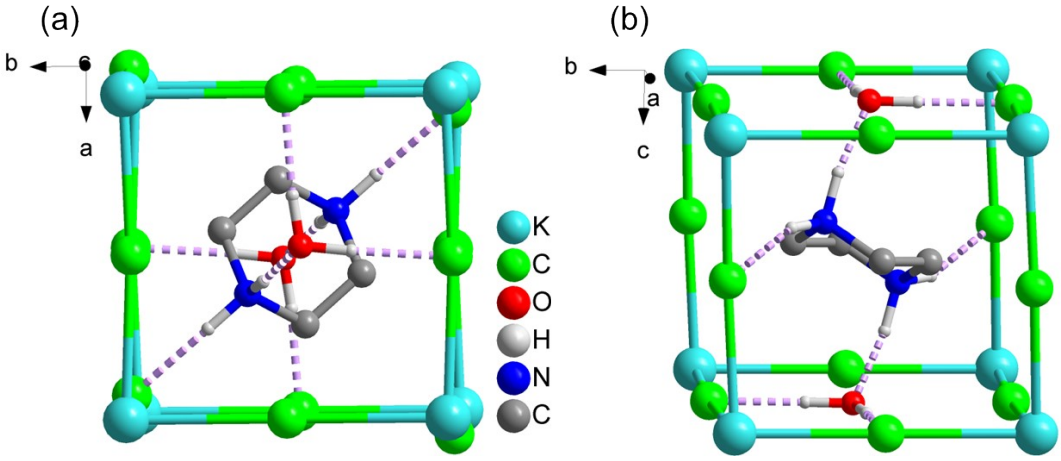

Figure S2. Hydrogen bond diagrams of $[C_4H_{12}N_2][KCl_3]\cdot H_2O$.

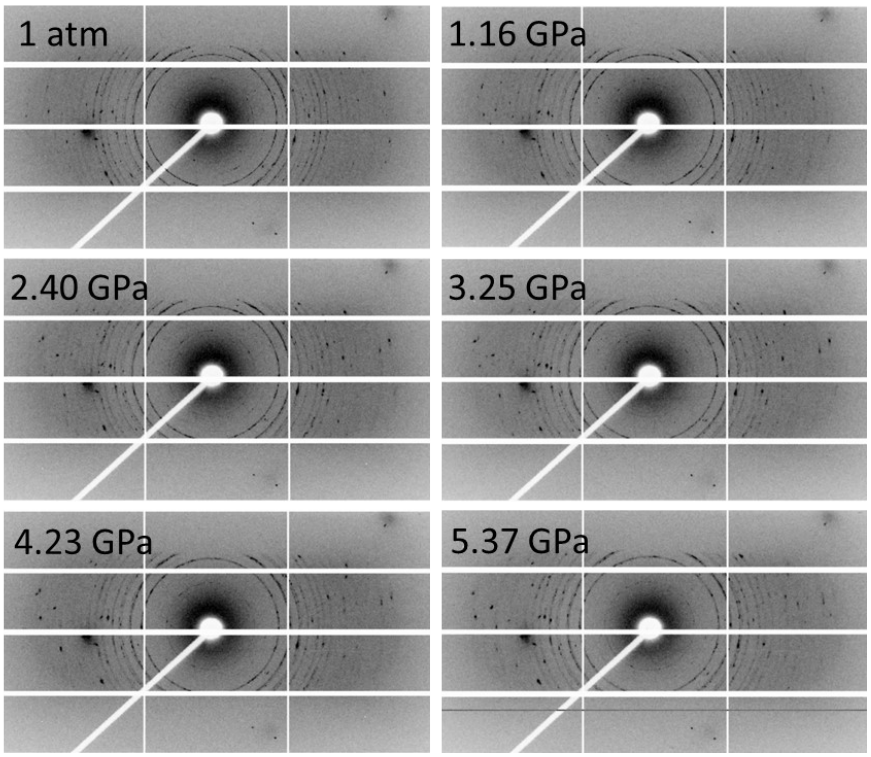

Figure S3. Representative 2D diffraction images at selected pressures of $[C_4H_{12}N_2][NH_4Cl_3]\cdot H_2O$.

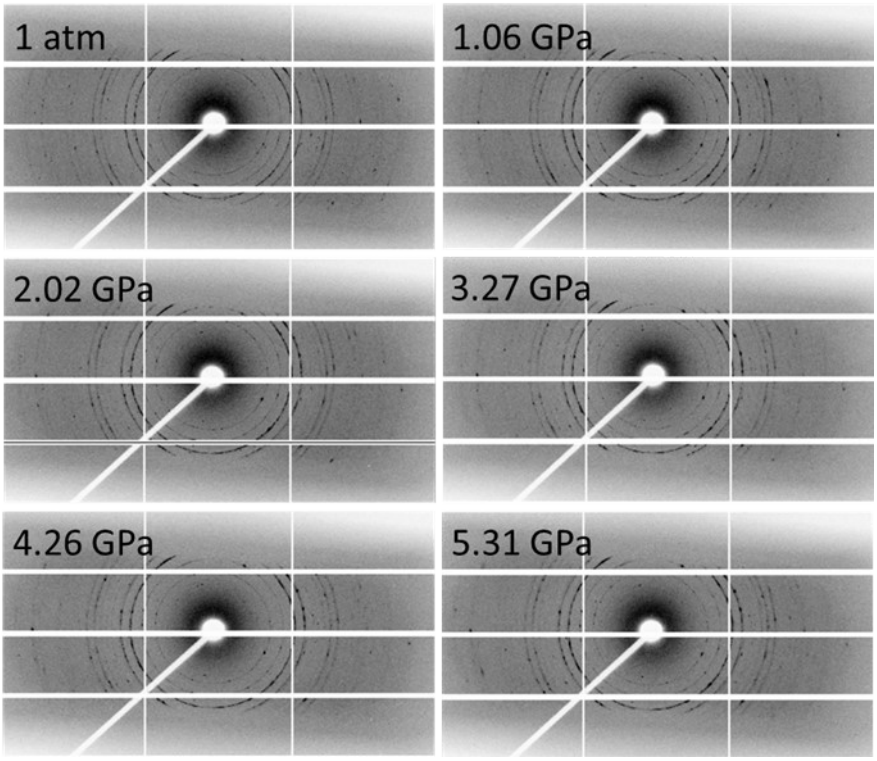

Figure S4. Representative 2D diffraction images at selected pressures of $[C_4H_{12}N_2][KCl_3]\cdot H_2O$.

References:

1. Li, K.; Dong, L.-Y.; Xu, H.-X.; Qin, Y.; Li, Z.-G.; Azeem, M.; Li, W.; Bu, X.-H., Electronic structures and elastic properties of a family of metal-free perovskites. *Mater. Chem. Front.* **2019,** *3* (8), 1678-1685.