Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Strong Enhancement of Second Harmonic Generation in Nonlinear Optical Crystals: 2-Amino-3-nitropyridinium Halides (Cl, Br, I)

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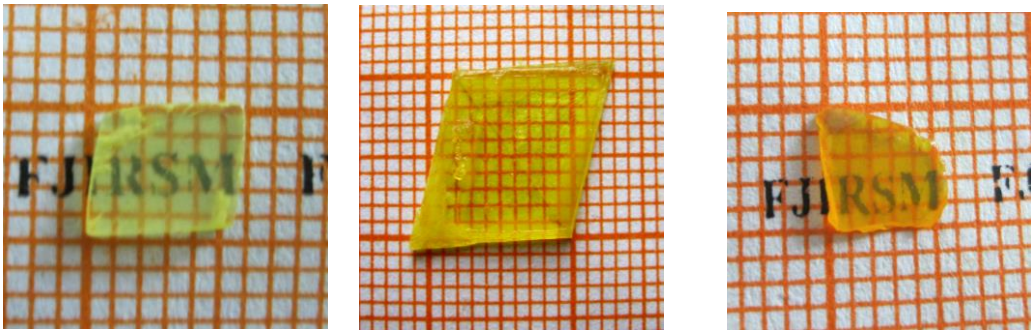
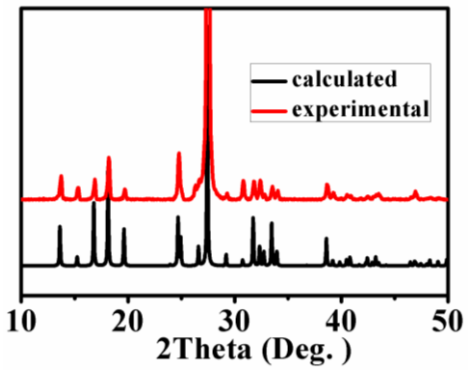
Supporting information

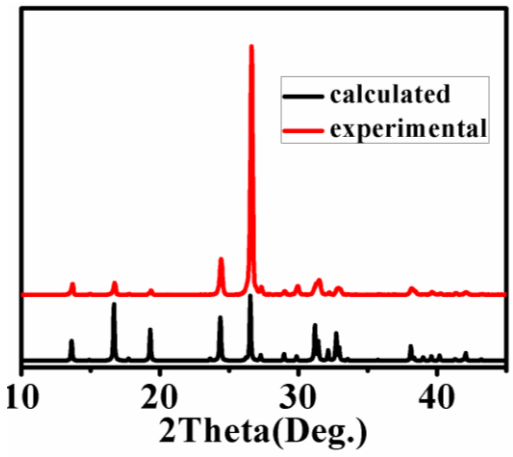


(a) (b) (c)

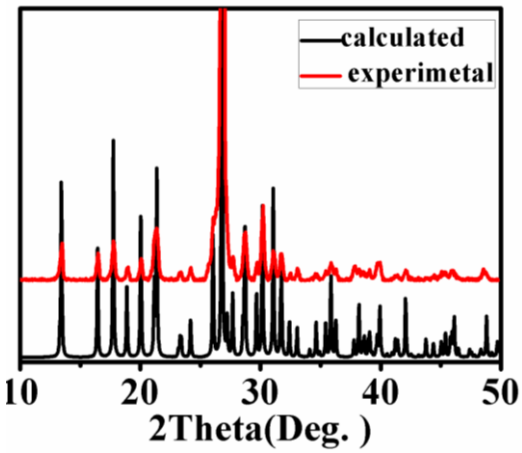
Figure S1. Photographs of crystal for (a) 2A3NPCl, (b) 2A3NPBr, (c) 2A3NPI



(a)



(b)



(c)

Figure S2. Experimental and caculated powder X-ray diffraction patterns for (a) 2A3NPCl, (b) 2A3NPBr, (c) 2A3NPI.

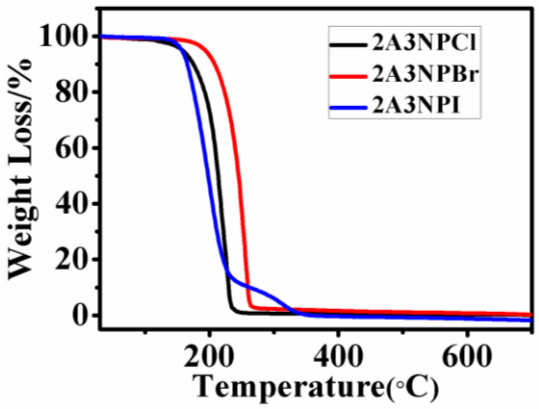


Figure S3. TGA curves of 2A3NPCl, 2A3NPBr and 2A3NPI.

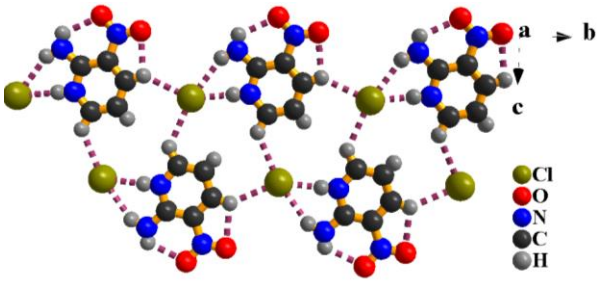


Figure S4. The anion-cation chain along b-axis of 2A2NPCl

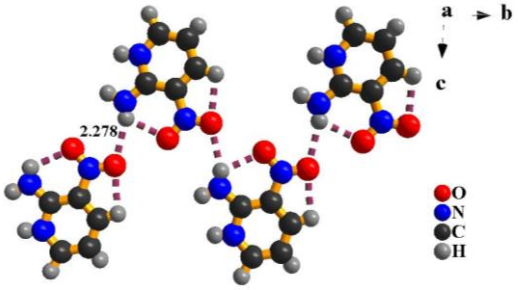


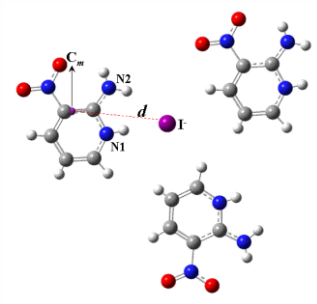
Figure S5. The zigzag chain by the unique intermolecular hydrogen bonds (N2−H2A···O2) extending along *c*-axis of 2A3NPCl.

Table S1. The calculated bond length and angles of hydrogen bonds in 2A3NPI by functional B3LYP with the 6-311+ G (d) mode.

	$d_{I\text{-}H1}$	$d_{I\text{-}N1}$	$d_{I\text{-}H2}$	$d_{I\text{-}N2}$	∠N1−H1···I	∠N2−H2···I
L4I	2.60438	3.46168	2.83303	3.63492	164.75895	152.21141
L3I	2.74247	3.59465	3.07529	3.91869	173.57058	157.44878

L4I: 2A3NPI

L3I: The molecular arrangement of 2A3NPI is supposed to be the same as that of 2A3NPBr as shown in the following caption.



L3I