Electronic Supplementary Material (ESI) for RSC Advances.

SUPPLEMENTARY MATERIALS

Widely Used Hardly Known.

An Insight into Electric and Dynamic Properties of Formamidinium Iodide

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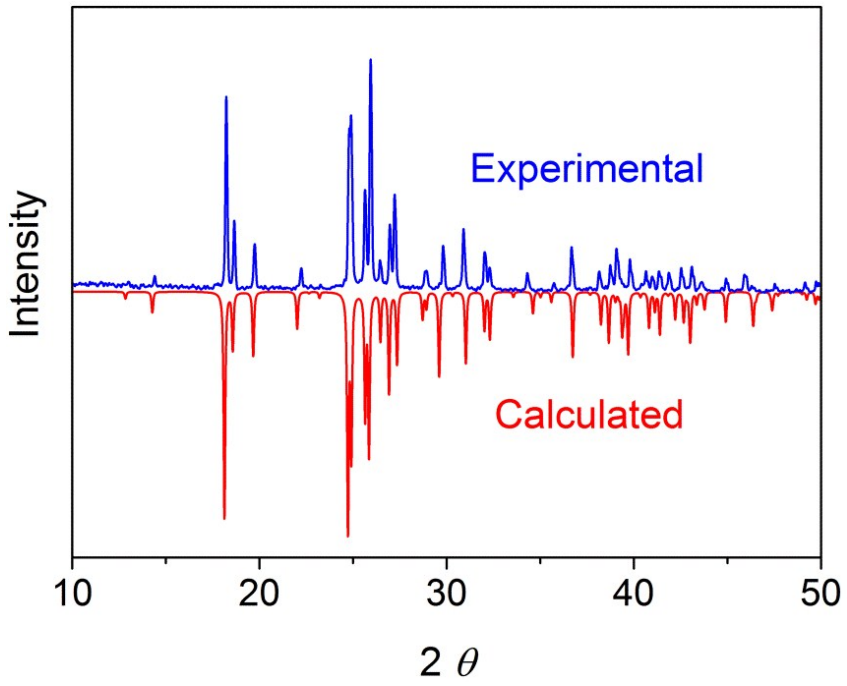

Figure S1. Calculated (red) and experimental (blue) X-ray powder diffraction data for **FAI**.

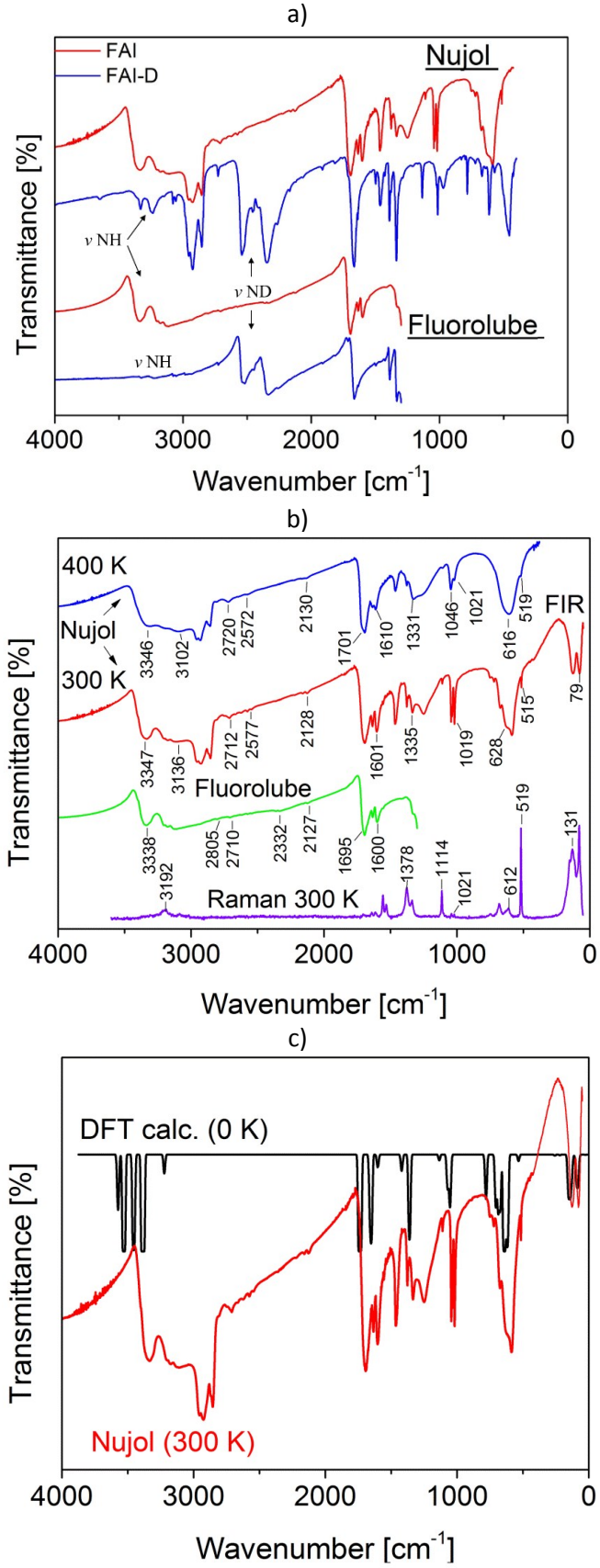

Figure S2.(a) The infrared spectra of the powdered **FAI** sample and **FAI-d** (deuterated sample); **(b)** The infrared spectra of the powdered **FAI** sample in Nujol (300 and 400 K) CsI, Fluorolube and FIR at 300 K and the FT-Raman spectra at 300 K; **(c)** Comparison of the calculated (black) and experimental (red) spectra for **FAI** crystal.

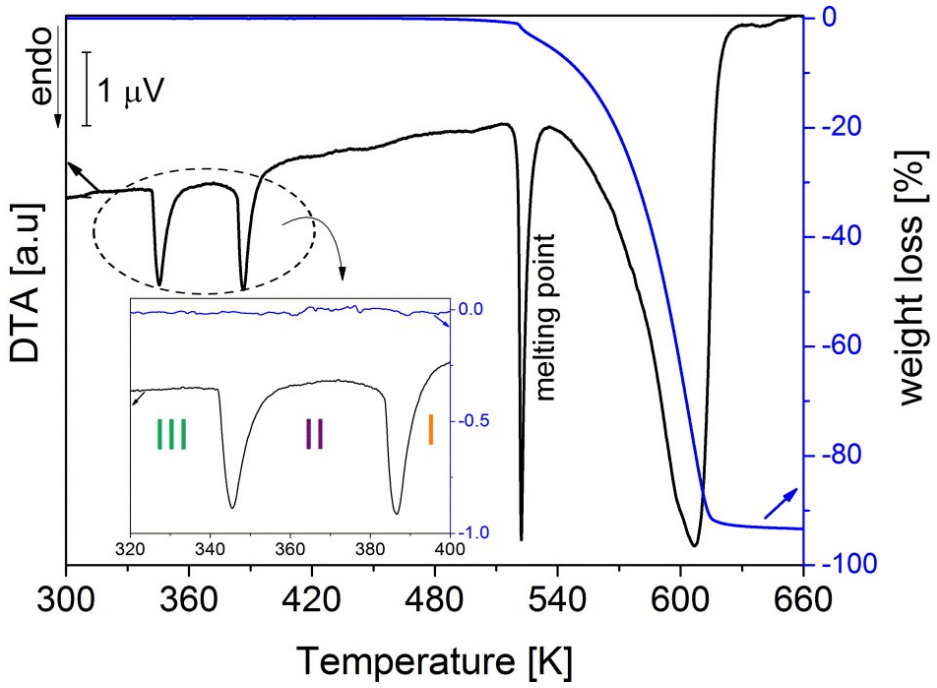

Figure S3. Simultaneous thermogravimetric and differential thermal analyses scan (ramp rate: 5 K min^{-1}).

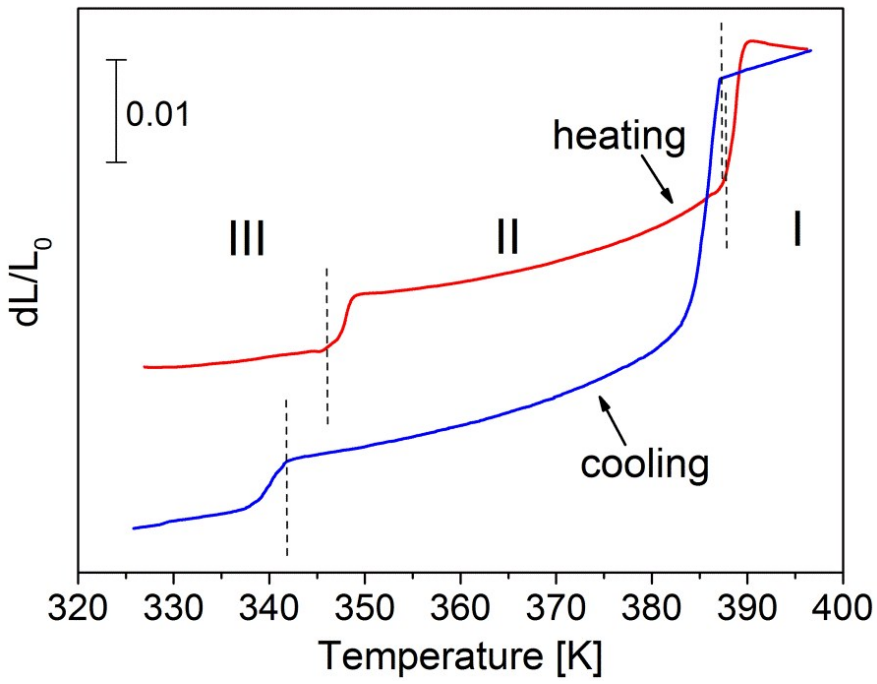

Figure S4. Dilatometric measurements for **FAI** (the scanning rate of 3 K min^{-1}).

Table S1. Comparison of the experimental and calculated selected vibrational frequencies in (cm^{-1}) for the **FAI**.

IR spectra				Assignments
In Nujol			DFT calc.	
T = 300 K	T = 350 K	T = 400 K	T = 0 K	
3398 w sh			3575	$\nu_{as}(NH_2)$
				$\nu_{as}(NH_2)$/νNH…I
3337 s	3336 s		3528	$\nu_{as}(NH_2)$/νNH…I
3310 s sh	3308 s sh	3320 s		
				ν_aNH_2/νNH…I
3203 s	3200 s	3199 vs		$\nu_{as}(NH_2)$/νNH…I
3176 s			3456	$\nu_s(NH_2)$/νNH…I
3129* vs				
3106 s	3103 s	3102 vs	3385	$\nu_s(NH_2)$
3112* vs				
			3223	ν(CH)
				ν(CH)
2984 vwsh				ν(CH)
2923* vs				ν(CH)
2852* vs				
2804* s				
2723 m				
2709 m	2714 m	2720 m		
2618 msh				
2577 m	2574 m	2572 m		
2547 m				
2222 w	2221 w	2224 w		
2161 w	2160 w	2162 w		
2128 w	2124 w	2130 w		
1695 vs	1698 vs	1701 vs	1745	$\nu_{as}(NCN) + \delta(NH_2) + \delta(CH)$
1676 s sh				
1636 s	1636 s	1636 s	1662	$\delta(NH_2)$
1601 vs	1606 vs	1610 s	1604	$\delta(NH_2) + \delta(CH)$
1557 m sh			1593	$\delta(NH_2)$+ δ(CH)
				$\delta(NH_2)$
1366 m	1365 m	1366 w	1417	$\nu_s(NCN)$
1335 m	1332 m	1331 m	1360	δ(CH)+ ν(C-N) + $\rho(NH_2)$
1306 m				
1249 s	1244 m	1256 m sh	1138	$\rho(NH_2)$
1170 w sh				
1157 w sh				
1110 w	1107 w	1105 vw		$\tau(NH_2)$
1044 s			1134	$\rho(NH_2)$
1036 s	1034 m	1046 m	1073	$\tau(NH_2) + \gamma(CH)$
1019 s	1014 m	1021 w	1051	$\rho(NH_2) + \delta(CH)+\gamma(CH)$
891 w sh				

894 vwsh				
722 vw	721 vw		761	$\tau(NH_2)$
673 m			673	$\tau(NH_2)$
623s sh			640	$\omega(NH_2)$
584 vs	600 vs	616 vs	620	$\omega(NH_2)$
515 m	514 w	519 w	534	$\tau(NH_2)(1.20)$
228 vw				
209 vw				
203 vw				
				lattice
127 vs				
79 s				
				vibrations
				trans. of I

* - in fluorolube; vs – very strong; s – strong, m – medium; w- weak; vw – very weak;sh-shoulder, ν-stretching vibration, δ-bending deformation in plane, τ-twisting deformation vibrations, ω-wagging deformation vibration, ρ-rocking deformation vibrations, γ-out-of-plane bending vibrations.