

Electronic Supplementary Information for

Explanation for the Selective Crystallization from Inosine Solutions using Mid-Frequency Raman Difference Spectra Analysis

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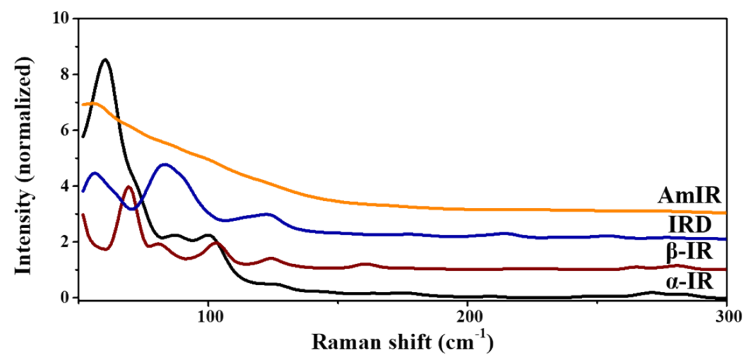


Figure S1. Low-frequency Raman spectra (LFRS, in the range of 50-300 cm^{-1}) of α -IR, β -IR, IRD, and AmIR.

Table S1. Characteristic shifts (cm^{-1}) of IR solids in the Low-frequency Raman spectra (LFRS, in the range of 50-300 cm^{-1}).

Polymorph	Characteristic shifts (cm^{-1})
α -IR	60, 88, 100
β -IR	69, 81, 103
IRD	56, 83, 123
AmIR	None

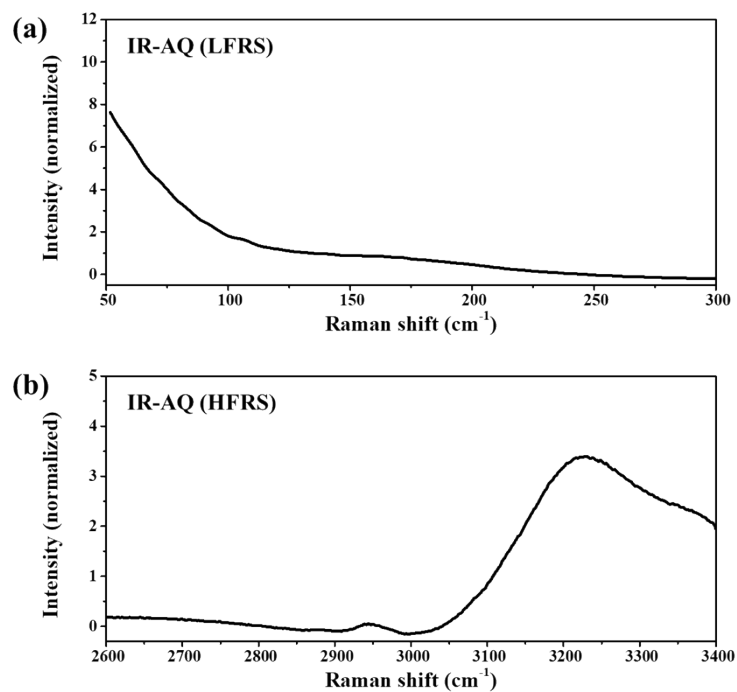


Figure S2. (a) LFRS and (b) high-frequency Raman spectrum (HFRS, in the range of 2600-3400 cm⁻¹) of IR-AQ.

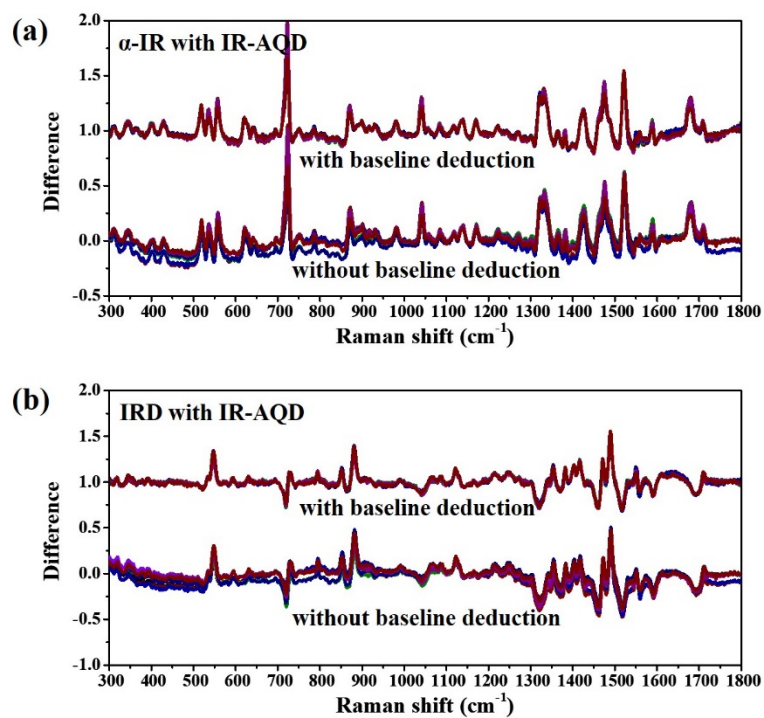


Figure S3. Mid-frequency Raman difference spectra (MFRDS) with and without baseline deduction of (a) α -IR and (b) IRD with IR-AQD. MFRDS with baseline deduction are shown with a translation on the vertical axis for clear. Each sample was characterized three times individually, and the corresponding nine MFRDS are shown here.

Table S2. Summary of the average deviation (a. d.) and standard deviation (s. d.) of all the data in the MFRDS without and with baseline deduction of IR samples with themselves. Each example was characterized three times individually, and the a. d. and s. d. were calculated from the corresponding three MFRDS.

MFRDS (300-1800 cm ⁻¹)	without baseline deduction		with baseline deduction	
	a. d.	s. d.	a. d.	s. d.
<i>self-α</i> -IR	0.015 (6)	0.026 (11)	0.012 (5)	0.020 (9)
<i>self-β</i> -IR	0.023 (7)	0.040 (13)	0.018 (6)	0.031 (10)
<i>self</i> -IRD	0.020 (6)	0.028 (8)	0.011 (4)	0.016 (5)
<i>self</i> -AmIR	0.014 (3)	0.017 (4)	0.007 (2)	0.010 (2)
<i>self</i> -IRAQD	0.052 (13)	0.062 (14)	0.013 (3)	0.017 (3)

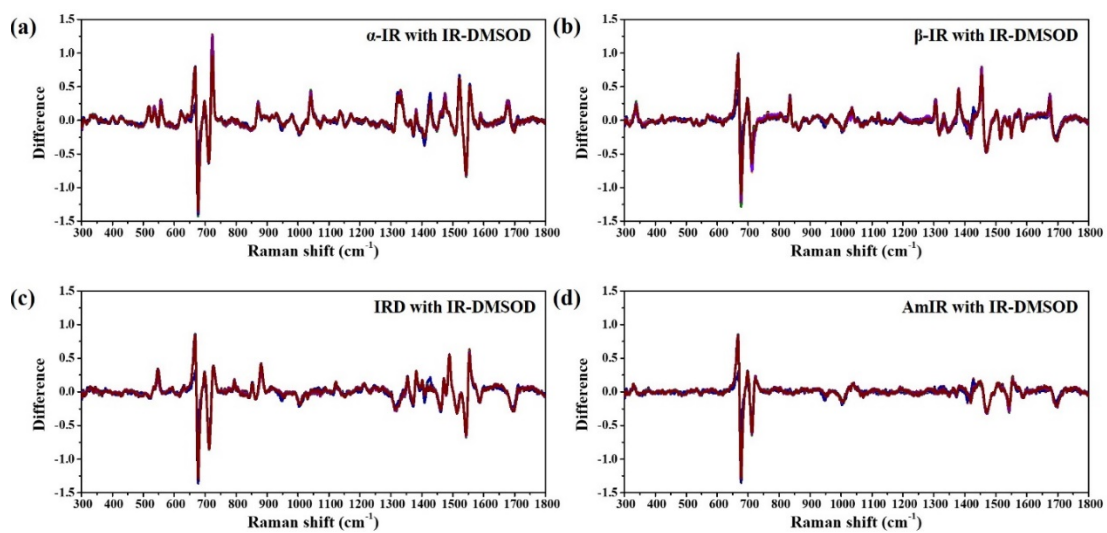


Figure S4. MFRDS with baseline deduction of (a) α -IR, (b) β -IR, (c) IRD and (d)

AmIR with IR-DMSOD.

Table S3. Summary of the a. d. and s. d. of all the data in the MFRDS with baseline deduction in different ranges (300-1800 cm^{-1} or 800-1800 cm^{-1}) of IR-DMSOD with itself. Example was characterized three times individually, and the a. d. and s. d. were calculated from the corresponding three MFRDS.

MFRDS with baseline deduction	300-1800 cm^{-1}		800-1800 cm^{-1}	
	a. d.	s. d.	a. d.	s. d.
<i>self</i> -IR-DMSOD	0.024 (13)	0.050 (32)	0.021 (10)	0.027 (13)