

# Supplementary Material: Understanding the Salt-Dependent Outcome of Glycine Polymorphic Nucleation

Guangjun Han, Pui Shan Chow and Reginald B.H. Tan

## Supplementary Materials—Properties and PXRDs of $\alpha$ -, $\beta$ - and $\gamma$ -glycine polymorphs

### 1. Properties of $\alpha$ -, $\beta$ - and $\gamma$ -glycine polymorphs

Some of the properties of the three glycine polymorphs are summarized in Table S1.

**Table S1.** Properties of  $\alpha$ -,  $\beta$ - and  $\gamma$ -glycine crystals.

Property	$\alpha$ -Glycine	$\beta$ -Glycine	$\gamma$ -Glycine
space group [1]	P2 <sub>1</sub> /n	P2 <sub>1</sub>	P3 <sub>1</sub> or P3 <sub>2</sub>
Z (formula units per cell) [1]	4	2	3
unit cell volume (Å <sup>3</sup> ) [1]	309.6	157.3	235.1
solubility in pure water at 298.15 K (g/(100g water)) [2]	25.03	NA	23.49
solution enthalpy $\Delta_{\text{sol}}H_{\text{m}}$ (J mol <sup>-1</sup> ) [3]	14,523 $\pm$ 76	14,198 $\pm$ 73	14,791 $\pm$ 84
sublimation enthalpy $\Delta H_{\text{sub}}$ at 298.15 K (J mol <sup>-1</sup> K <sup>-1</sup> ) [4]	140.58	138.09	141.70
isobaric heat capacity $C_p$ at 298.15 K (J mol <sup>-1</sup> K <sup>-1</sup> ) [4]	89.85	90.46	89.78

### 2. PXRD patterns and analyses of glycine polymorphs

The simulated PXRD patterns of  $\alpha$ -,  $\beta$ - and  $\gamma$ -glycine references are shown in Figure S1-a. Note that Materials Studio's CSD codes of Gly29 ( $\alpha$ -form), Gly33 ( $\gamma$ -form) and Gly31 ( $\beta$ -form) were used in PXRD simulation. As an illustration of solid phase analyses, the PXRD patterns of  $\alpha$ -glycine crystal samples before and after the test of  $\alpha$ -glycine solubility in a glycine aqueous solution in the presence of 1m Na<sub>2</sub>SO<sub>4</sub> are presented in Figures S1-b. Similarly, the PXRD patterns of  $\gamma$ -glycine crystal samples before and after the test of  $\gamma$ -glycine solubility in a glycine aqueous solution in the presence of 1m Na<sub>2</sub>SO<sub>4</sub> are presented in Figures S1-c.

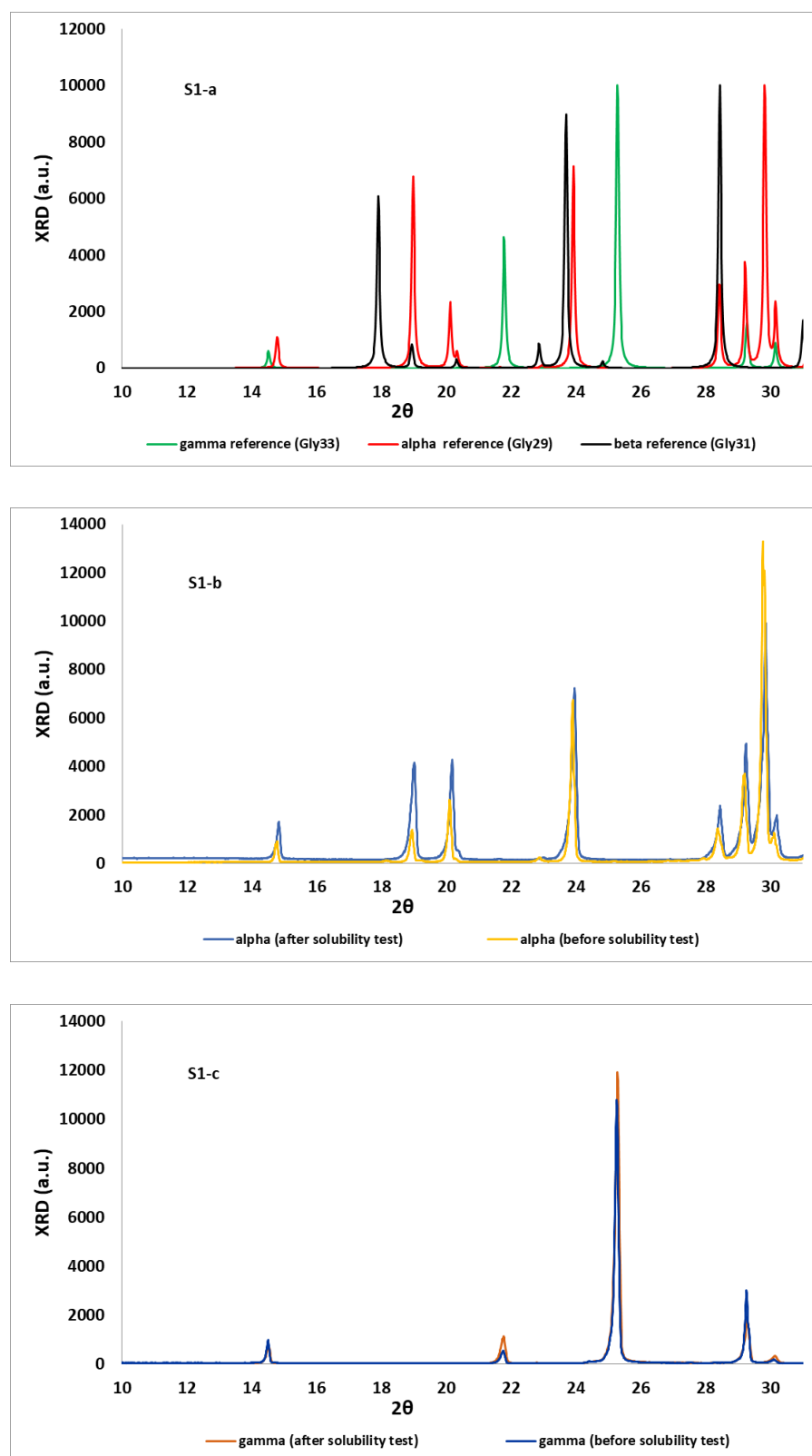
Comparing the PXRD patterns (Figure S1-b) of  $\alpha$ -glycine crystal samples with those (Figure S1-a) of  $\alpha$ -,  $\beta$ - and  $\gamma$ -glycine references reveals that the metastable  $\alpha$ -glycine crystals remained unchanged in their polymorph before and after  $\alpha$ -glycine solubility test through an isothermal method. In a similarly way, comparing the PXRD patterns (Figures S1-a and S1-c) enables us to conclude that the thermodynamically stable  $\gamma$ -glycine crystals (Figure S1-c) also remained unchanged in their polymorph before and after  $\gamma$ -glycine solubility test, which is well expected.

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**Figure S1.** PXRD patterns of  $\alpha$ -,  $\beta$ - and  $\gamma$ -glycine references (S1-a),  $\alpha$ -glycine crystal samples (S1-b) before and after the  $\alpha$ -glycine solubility test, and  $\gamma$ -glycine crystal samples (S1-c) before and after the  $\gamma$ -glycine solubility test.

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## References

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