

Understanding Growth Morphology Changes of γ -Glycine and DL-alanine Polar Crystals in Pure Aqueous Solutions

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TITLE RUNNING HEAD: Unexpected Changes in Growth Morphology of Polar Crystals

Supporting Information (Manuscript ID: cg-2010-00934f) – Using PXRD and Raman spectrometry to determine the polymorphic purity of γ -glycine and α -glycine

We have obtained the PXRD patterns of the glycine seed crystals we made and we have reported them in Figure 1 (for γ -glycine) and Figure 2 (for α -glycine). Given that the PXRD patterns of our glycine samples are in very good agreement with the simulated diffraction patterns¹ and the reference PXRD

patterns¹ of γ -glycine (cf. Figure 1) and α -glycine (cf. Figure 2) respectively, we confirm that our glycine samples were a powder of either pure γ -glycine or pure α -glycine, not a mixture of polymorphs. These pure γ -glycine and α -glycine powders were then used to establish the distinct Raman spectra (cf. Figure 3) of γ -glycine and α -glycine respectively for distinguishing and identifying the polymorphic form of a single glycine seed crystal^{2,3} prior to its growth in a solution.

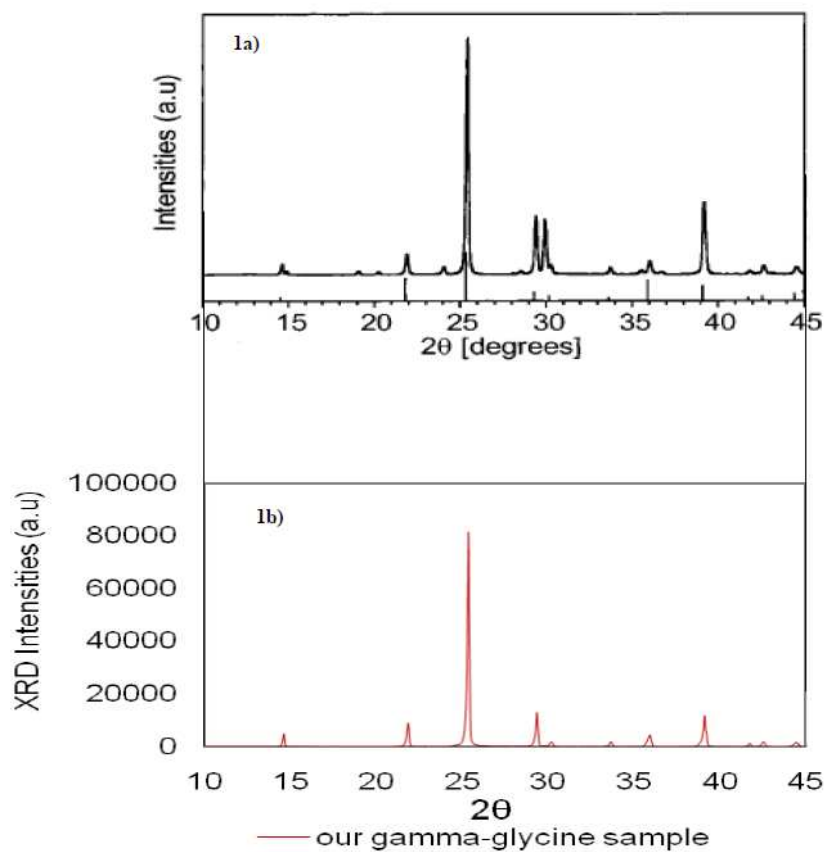


Figure 1. 1a) Simulated diffraction pattern (represented by sticks) and reference PXRD pattern of a pure γ -glycine sample (Cryst. Growth Des. **2001**, 1, 5–8); 1b) PXRD pattern of our γ -glycine sample.

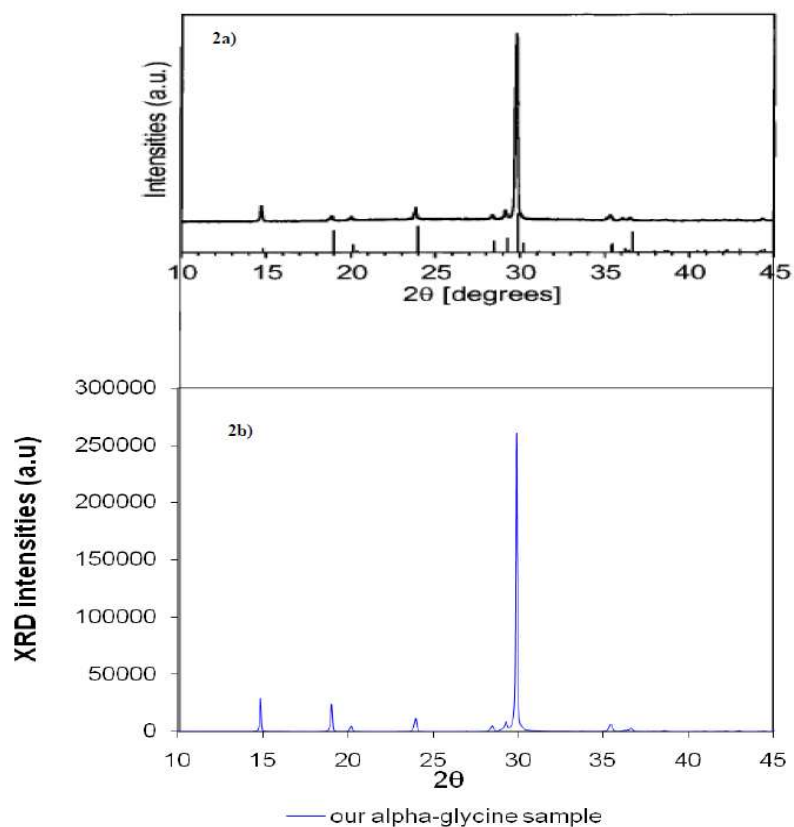


Figure 2. 2a) Simulated diffraction pattern (represented by sticks) and reference PXRD pattern of a pure α -glycine sample (Cryst. Growth Des. **2001**, 1, 5–8); 2b) PXRD pattern of our α -glycine sample.

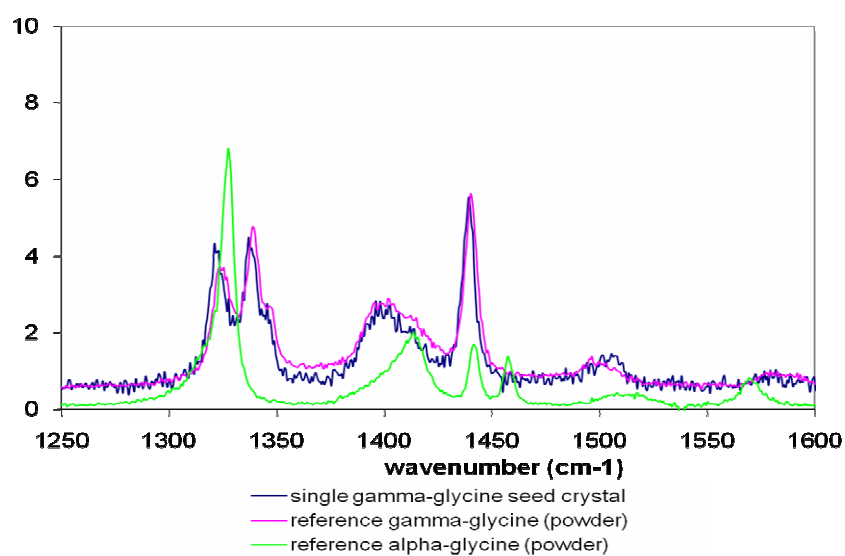


Figure 3. Raman spectra of reference α - and γ -glycine (powder) and a single γ -glycine seed crystal.

REFERENCES

1. Zaccaro, J.; Matic, J.; Myerson, A. S.; Garetz, B. A. Cryst. Growth Des. **2001**, 1, 5–8.
2. Lee, A. Y.; Lee, I. S.; Myerson, A. S. Chem. Eng. Technol. **2006**, 29, 281–285.
3. Lee, I. S.; Kim, K. T.; Lee, A. Y.; Myerson, A. S. Cryst. Growth Des. **2008**, 8, 108–113.