

Structure of Glycine Dihydrate: Its Implications to Crystallization of Glycine from Solution and Modification of Glycine in Space

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Abstract: Glycine, the simplest amino acid, is also the most polymorphous. Herein, we report the structure determination of an unknown phase of glycine which was firstly reported by Pyne and Suryanarayanan in 2001. To date, the new phase has only been prepared at 208 K as nanocrystals within ice. Through computational crystal structure prediction and powder X-ray diffraction methods, we identified this elusive phase as glycine dihydrate (**GDH**), representing the first report on a hydrated glycine structure. The structure of **GDH** has important implications for the state of glycine in aqueous solution, and the mechanisms of glycine crystallization. **GDH** may also be the form of glycine that comes to Earth from extraterrestrial sources.

