

The Energetics of Amino Acid Synthesis and Polymerization as a Function of Temperature and pH.

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Introduction: Since their discovery in the late 1970s, submarine hydrothermal systems have been proposed as likely candidates for the origin and evolution of life on Earth [1]. In hydrothermal systems, seawater percolates into the oceanic crust and is heated, reacting with surrounding rocks. The resultant hot reductive fluid shows pH ranging from <1 to 11 and temperatures from 2 to 400 °C. To evaluate the potential for abiotic organic synthesis under such hydrothermal conditions, thermodynamic calculations have been performed widely [2]. However, most of previous calculations have been performed assuming neutral pH. Reactivities of organic molecules under other pH conditions remain not well known. Therefore in this study, I performed thermodynamic calculations for the synthesis and polymerization of amino acids (especially glycine (Gly)) under wide range of temperature (0-300 °C) and pH (2-12) conditions.

Results and Discussion: Figure 1 shows the standard molal Gibbs energies ($\Delta_r G^\circ$) of formation ($2\text{CO}_2 + \text{NH}_3 + 3\text{H}_2 \rightarrow \text{Gly} + 2\text{H}_2\text{O}$; Fig. 1a) and dimerization ($\text{Gly} + \text{Gly} \rightarrow \text{GlyGly} + \text{H}_2\text{O}$; Fig. 1b) of Gly as a function of temperature and pH. In both the cases, strong temperature and pH dependences are observed. For instance at pH = 6, the values of $\Delta_r G^\circ$ for Gly formation increased with increasing temperature (Fig. 1a), whereas those of Gly dimerization decreased (Fig. 1b). These results indicate that favorable environments for the formation and polymerization of Gly are different; lower temperature and neutral pH condition is favorable for Gly formation whereas higher temperature and slightly alkaline (or slightly acidic) pH is favorable for Gly polymerization (neutral pH at 300 °C is ~5.4). Therefore, formation and polymerization of amino acids might proceeded under different hydrothermal environments on the primitive Earth.

References:

- [1] Takai K. et al. (2006) *Paleontol. Res.*, 10, 269.
- [2] Amend J. P. et al. (2013) *Phil. Trans. R. Soc. B*, 368, 1.

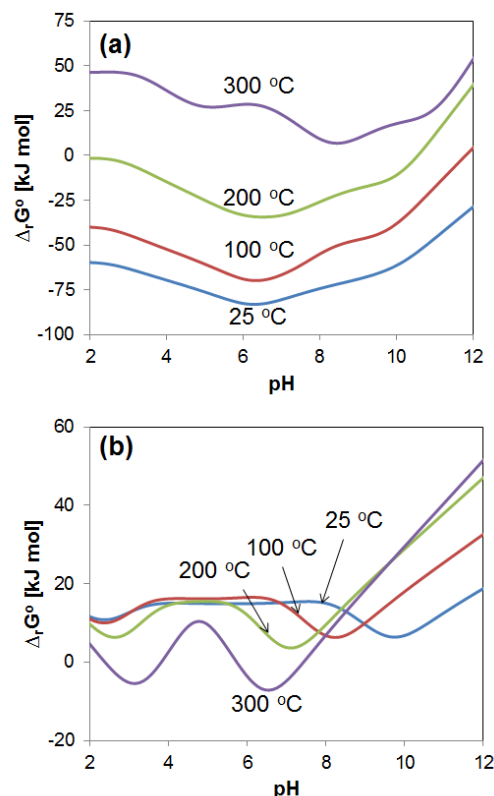


Figure 1. Standard molal Gibbs energies ($\Delta_r G^\circ$) of formation ($2\text{CO}_2 + \text{NH}_3 + 3\text{H}_2 \rightarrow \text{Gly} + 2\text{H}_2\text{O}$; Fig. 1a) and dimerization ($\text{Gly} + \text{Gly} \rightarrow \text{GlyGly} + \text{H}_2\text{O}$; Fig. 1b) of Gly as a function of temperature and pH.