Quantifying the Extent of Amide and Peptide Bond Synthesis Across Conditions Relevant to Geologic and Planetary Environments (2021)

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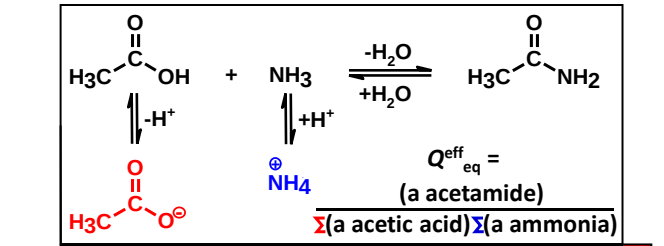
H ydrothermal O rganic G eochemistry

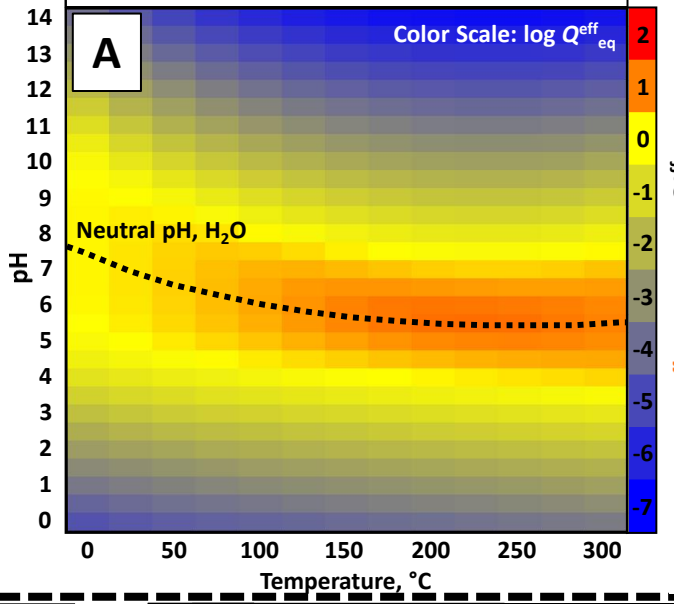
To gain an understanding of the critical parameters controlling amide and peptide bond formation in natural systems, we used thermodynamic calculations to assess the effects of temperature, pH, and pressure on aqueous amide synthesis.

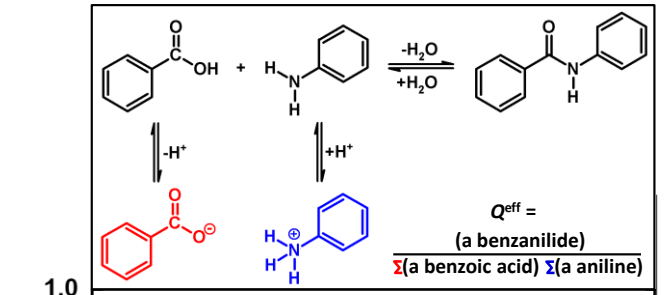
As a simple example, we explored the reaction of acetic acid and ammonia to form acetamide, while also taking into account pH effects on the aqueous speciation of the reactants. This allowed us to calculate effective reaction quotients (Q^{eff}_{eq}, color scale), for which greater values favor amide formation.

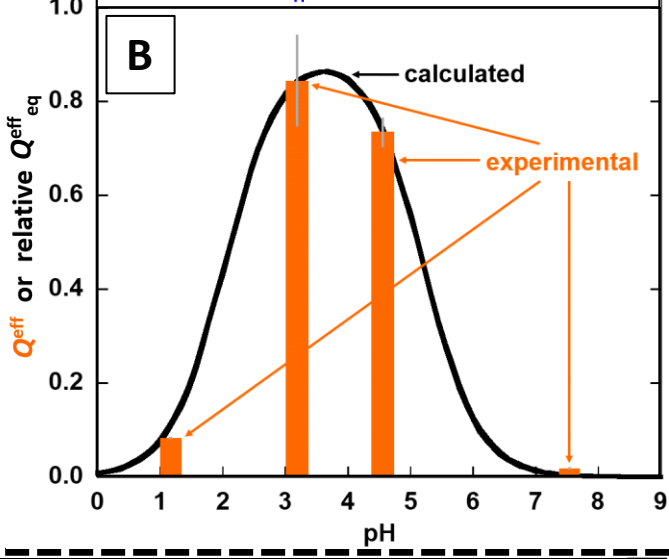
We found that acetamide formation is most favorable (red region, **A**) under hydrothermal conditions at circumneutral pH.

Our model is supported by analogous experiments at a subset of conditions (**B**).









We applied the same modeling strategy as above to identify optimal synthesis conditions for a peptide bond in water, which involves a slightly more complex set of reactions.

We modeled diglycine formation from two glycine molecules across the same ranges of temperature and pH (**C**), and also produced a model at high pressure (30 kbar, **D**).

Our results suggest that glycine synthesis is more favorable at higher temperatures nearer ambient pressures, but more favorable at lower temperatures at high pressures.