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Thermodynamic Calculation of the Relative Stabilities of Enzymes, DNA, and Other Biomacromolecules Under Extreme Conditions of Temperature and pH

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Combining computed equilibrium constants for protein unfolding at temperatures from 238.l5 to 473.15 K with extrapolated values of the difference in the mean net charge of the unfolded and folded protein species as a function of pH permits calculation of the degrees of formation of enzymes in and beyond the regions of temperature and pH in which extremophiles are currently known to thrive in geologic systems. This approach permits investigation of the factors responsible for enzyme stability under these extreme conditions. The calculations were carried out using a modified and updated version of the SUPCRT92 software package called OBIGT01 by taking explicit account of the static dielectric constant of supercooled water from 238.15 to 273.15 K (Fernandez et al., 1995). The computed degrees of formation indicate that enzymes may be psychrophilic and/or thermophilic at either or both extremes of pH, depending on the size and relative populations of charged and neutral exterior and interior side chains. Cold denaturation may or may not occur in the intermediate pH region, depending on the protein. Consideration of similarities in the thermodynamic behavior of protein unfolding and DNA melting suggests that DNA (and by inference other biomacromolecules) should also be stable at extremes of pH and temperature. The predictions of the relative stabilities of acidophilic enzymes are consistent with the reported optimal growth temperature and pH for the new archea with the suggested name *Ferroplasma acidarmanus* discovered recently by Edwards et al. (2000). The calculations also indicate that the acidophilic enzymes required to support microbial life should be stable relative to their unfolded counterparts at pHs as low or lower than those reported by Nordstrom and Alpers (1999) for Iron Mountain acid mine waters (0.48 to -3.6). In fact they strongly support from a thermodynamic perspective the notion that life may exist in geologic systems at both extremes of pH at temperatures well above those that have been documented to date, perhaps as high or higher than 473.15 K.

Fernandez DP, Mulev Y, Goodwin ARH & Levelt Sengers JMH, *J. Phys. Chem. Ref. Data*, **24**, 33-69, (1995).

Edwards KJ, Bond PL, Gihring TM & Banfield JF, *Science*, **287**, 1796-1799, (2000).

Nordstrom DK & Alpers CN, *Proc. Natl. Acad. Sci. USA*, **96**, 3455-3462, (1999).