Energetics of Biological Macromolecules from Five-Dimensional Crystallographic Data

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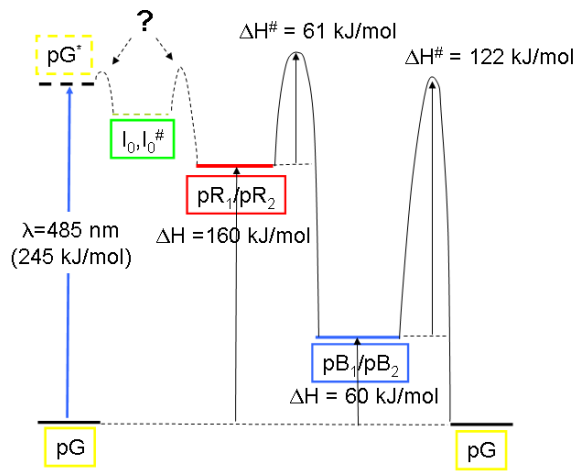

Energetics of the photoactive yellow protein. Activation enthalpies ($\Delta H^{\#}$) from 5-D crystallographic data. Enthalpies of pB and pR relative to pG from Takeshita, Hirota, Imamoto and Kataoka (2001), Analytical Sciences, v17, s320-s322.

Arrhenius plots from 5-dimensional crystallographic data provide enthalpy and entropy values of transition states. In five-dimensional crystallography [1] time *and* temperature is also taken into consideration in addition to space and an analysis based on singular value decomposition [2] is applied. We present results of such a time-resolved crystallographic study. Temperature dependent time-resolved X-ray diffraction measurements were conducted at the newly upgraded BioCARS 14-ID-B beamline at the Advanced Photon Source. The measurements aimed at elucidating a comprehensive kinetic mechanism of the photocycle of the photoactive yellow protein including enthalpy and entropy values of all rate coefficients in concert with the atomic structures of the transient intermediates. Comprehensive time-series of crystallographic data were collected at four temperatures, 10°C, 20° C, 25°C and 30° C. Relaxation times extracted by singular value decomposition from these time-series exhibit measurable differences for the temperatures. Arrhenius plots from these data demonstrate that five-dimensional crystallography is feasible.

[1] Schmidt, Graber, Henning, Srajer (2010) Five-Dimensional Crystallography, Acta Cryst A, 66, 198-206.
[2] Schmidt, Rajagopal., Ren, Moffat (2003) Application of Singular Value Decomposition to the Analysis of Time-Resolved Macromolecular X-ray Data. Biophys. J. 84 2112-2129