Energy Storage and Transport in Proteins. Förner, W.

Abstract

Energy which is injected into protein α-helices by biological processes such as ATP (Adenosinetriphosphate)

hydrolysis excites a vibration of relatively high energy, namely the amide-I vibration which consists mainly

of C=O stretch. The energy released by ATP hydrolysis is roughly 0.4 eV, while two amide-I vibrational

quanta correspond to 0.41 eV. The C=O groups in an α-helix are involved in hydrogen bonding to the N-H

groups in the next helical turn. This interaction basically stabilizes the α-helical structure. Thus there are three

chains of hydrogen bonded C=O…H-N groups parallel to the helix axis. Two neighboring C=O groups along

such a chain are coupled by their dipole moment. This gives rise to an interaction which would cause a

vibrational excitation at one C=O group to disperse through the complete chain in its extended normal modes.

Thus in this way the energy seemingly could not be stored or transported in an α-helix, besides the near perfect

match of the energies involved.

However, the hydrogen bonded peptide groups in this chain can vibrate against each other. These lattice vibrations, or phonons when quantized, are of very low energy compared to the amide-I vibration. What they actually do is that they change the length of hydrogen bonds in which the C=O groups are involved. If the length of a hydrogen bond changes, also the vibrational energy of the C=O vibration involved in the hydrogen bond changes. Thus there is an interaction between the amide-I vibration and the lattice phonons. Further, this interaction appears as a nonlinear term in the equations of motion for the amide-I vibrational quanta. And as usual, these nonlinear interactions have a localizing effect on the amide-I quanta.

In other words, an amide-I vibration when excited would not disperse, because via the nonlinear interaction it distorts the chain around it in such a way that a potential wall against dispersion is created. If the strength of the dispersive force (dipole interactions between the C=O groups) and the nonlinear force are balanced, then the dispersive force still would cause the amide-I quantum to move while the nonlinear force prevents it from actual dispersion. Thus the amide-I quantum would move through the α-helix just like a particle through space, carrying its lattice deformation with it. Such a structure is called a Davydov soliton.