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An essay on the role of the hydrogen bonding structures for long range interactions in proteins monitored in the far infrared

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In order to understand the molecular basis of energy transduction, our group has extensive interest in developing experiments which reveal at the molecular level how protons are drawn through proteins. It is not only essential to determine the local pK value of the crucial amino acid side chains and to define the structural, dynamic and energetic requirements for the proton transferring groups, a significant part of the proton conduction is made by channels that orient specifically bound water molecules. Long range signalling is observed in all transmembrane proteins, including those that transport protons. We aim to monitore these interactions on the basis of the hydrogen signature in the far infrared and analyse the specificity of this spectral range. The use of synchrotron bases sources is presented.

The experiments discussed, include far infrared spectroscopic studies on the hydrogen bonding signature of complexes III and IV from the respiratory chain in function of temperature. The following examples presented.

i) Complex IV, the so called cytochrome *c* oxidase, the molecule that catalyses the reduction of oxygen to water and couples this process to the pumping of protons. An interesting effect is investigated, namely a residue, located 20 A away from the active side, that uncouples the oxygen reduction from proton pumping via the water channel[1].

ii) Complex III, performs a large conformational change during its catalytic cycle. This change and thus the catalytic cycle can be inhibited with so called Stigmatellin. Far infrared data was used to monitor the change in internal reorganisation of the protein upon inhibition and the involvement of the water channel from the outside to the active side.

Reference

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