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WATER-INDUCED REVERSIBLE CONFORMATIONAL CHANGE IN DEOXYHEMOGLOBIN

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Our aim is the study of the role played by the water in the structure and function of hemoglobins (Hb). Here we present results obtained by visible absorption spectroscopy of deoxy-Hb films kept in an oxygen-free environment with a varying degree of hydration. An oxy-Hb solution in a closed cuvette was deoxygenated by vacuum and the formation of the deoxy derivative was observed visually by the change of the solution color to purple. As the evacuation continued, a dry film was obtained on one of the cuvette walls. The absorption spectrum of this film showed bands at 425 (Soret's band), 530 and 559 nm, characteristic of the hemochrome derivative. The film was then exposed to an environment containing deoxygenated water. As water was absorbed by the protein, there was a decrease in the intensity of the characteristic hemochrome bands and the appearance of a band at 555 nm, typical of the deoxy-Hb. This transformation could also be followed in Soret's band. Upon subjecting the film to a water sorption-water desorption process in the absence of O_2, we observed that the process

$$\text{hemochrome} \underset{-H_2O}{\overset{+H_2O}{\rightleftharpoons}} \text{deoxy-Hb}$$

is reversible. We noticed also that, in contact with O_2, the hydrated film was transformed to oxy-Hb. From these experiments we conclude that upon dehydration the deoxy-Hb undergoes a structural rearrangement in the heme region, which allows the binding of the histidine E7 to the Fe ion (hemochrome structure). Also, the removal of the hydration water does not change the oxidation state of the Fe ion; therefore, the rehydrated protein preserves its ability to reversibly bind O_2.

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