those obtained for interlayer and interchain distances and for the width of the main phase transition calorimetric peak. At the highest dose (~80 kGy) molecules of cross linked adjacent radicals and other molecular species are also formed. Appreciable differencies, with some similarities, were observed in the behaviour of DSPC and DPPC liposomes under γ-irradiation.

02.10-1 CALCULATION OF THE VIBRATIONS OF HELICAL STRUCTURES IN POLYPEPTIDES.

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In the last few years there has appeared a number of experimental reports and theoretical analyses concerning the low-frequency motions in biomacromolecules. Brown et al. /1/ observed that low-frequency Raman bands exist in certain proteins, and these vibrations appeared to be sensitive to the conformation of a protein. Among the component elements of protein molecules helices occupy a prominent position.

For the theoretical investigation of vibrations of helical structures in proteins, we have used a molecular mechanics procedure to calculate the total energy including the energy contributions of the $C_i{=}O_i \ldots H_{i+n}{-}N_{i+n}$ (n = 3, 4) H-bonds of a polyglycine helix model depending on the dihedral angles φ, ψ forming regular helical structures. We have additionally calculated the following geometrical parameters of this helix model depending on φ-, ψ-angles:

(i) the length per residue of the helix - 2SH (Å),

(ii) the angle of winding of the helix - WDG (deg.),

(iii) the H-bond distances $d_n{=}O_i \ldots H_{i+n}$ (n = 3, 4),

(iv) the H-bond angles $\omega_n{=}C_i{=}O_i \ldots H_{i+n}$ (n = 3, 4) and

(v) the H-bond angles $\eta_n{=}O_i \ldots H_{i+n}{-}N_{i+n}$ (n = 3, 4).

The calculated energy surface allows to define a "low energy pathway" (LEP) in the φ,ψ-plane along which the vibrations of the regular polyglycine helix can take place. The changes of all the geometrical helical parameters (i)-(v) along the LEP enable us to give the following interpretation of the vibration of this helix model. The vibration of the helix can be divided into two regions along the LEP.

In the first region from A (φ_A = -72.0°, ψ_A = -17.0°) up to B (φ_B = -71.5°, ψ_B = -32.5°) on the LEP the helix performs a longitudinal and a torsional vibration.

In the second region from B up to C (φ_C = -33.5°, ψ_C = -71.5°) on the LEP the helix changes only the steric orientation of the peptides relative to the helix axis depending on the alteration of φ-, ψ-angles (and in this connection, changes of the H-bond geometry). But there is no longitudinal and only a minor torsional vibration in this second region.

/1/ Brown, K.G., Erfurth, S.C., Small, E.W. & Perticolas, W.L.L. (1972) Proc. Natl. Acad. Sci. U.S.A. 69, 1467-1469.

02.10-2 CATALYSIS IN THE CRYSTAL: SYNCHROTRON RADIATION STUDIES WITH GLYCOGEN PHOSPHORYLASE b.

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Direct observation of the progress of a catalysed reaction in crystals of glycogen phosphorylase b has been made possible through fast crystallographic data collection achieved at the Synchrotron Radiation source at Daresbury. In the best experiments, data to 2.7Å resolution (some 108,300 measurements; 21,200 unique reflections) were measured in 25 mins. In a series of time resolved studies in which the control properties of the enzyme were exploited in order to slow down the reaction, the conversion of heptenitol to heptulose-2-phosphate, the phosphorylysis of maltoheptaose to yield glucose-1-phosphate and the oligosaccharide synthesis reaction involving maltotriose and glucose-1-phosphate have been monitored in the crystal. Changes in electron density in the difference Fourier maps are observed as the reaction proceeds not only at the catalytic site but also the allosteric and glycogen storage sites. Phosphorylase b is present in the crystals in the T state and under these conditions exhibits low affinity for both phosphate and oligosaccharide substrates. However there are pronounced conformational changes associated with the formation and binding of the high affinity deadend product, heptulose-2-phosphate, which show that movement of an arginine residue, Arg569, is critical for formation of the substrate-phosphate recognition site. Recent results from the refinement of the ligand complexes will be discussed.