

**02.6-02** PORIN (MATRIX PROTEIN) FROM *E. COLI*. STRUCTURE OF TWO-DIMENSIONAL CRYSTALLINE SHEETS BY ELECTRON MICROSCOPY AND ELECTRON DIFFRACTION. By D. L. Dorset, A. Engel and J. P. Rosenbusch, Microbiology Department, Biozentrum, University of Basel, Klingelbergstrasse 70, Basel, Switzerland.

Electrical measurements on planar lipid membranes containing porin (Schindler and Rosenbusch, Proc. Nat. Acad. Sci. (1981) in press) have shown that this protein of *E. coli* outer membrane may be regarded as a paradigm of pore-forming transmembrane proteins. Two-dimensional crystalline arrays, reconstituted with dimyristoyl lecithin and negatively stained with uranyl acetate, have been found to give electron diffraction patterns with resolution to about 20 Å. Computer reconstruction of electron images from untilted specimens reveal the structure to be similar to the two-dimensional sheets previously obtained by detergent extraction (Steven, et al, J. Cell Biol. (1977) 72, 292). Electron diffraction intensity distributions along reciprocal lattice spikes, obtained from several tilt series, confirm that the space group is trigonal (P3), with  $a = 92 \text{ \AA}$ . The membrane sheet thickness is about 50 Å. In order to correlate the protein packing in these sheets with x-ray structure determinations on two three-dimensional crystalline forms (Garavito and Rosenbusch, J. Cell Biol. (1980) 86, 327, and unpublished), three-dimensional reconstructions are made using data from tilt series to  $\pm 45^\circ$ .

**02.6-03** THE CONFORMATION OF THE FIRST SEGMENTS IN THE FATTY ACYL CHAINS OF 3-SN AND 2-SN<sub>2</sub> PHOSPHOLIPIDS. G. Büldt, J. Seelig and G.H. de Haas.  
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Extensive work has been reported on the conformation in membranes of 3-sn-phosphatidylcholines, -ethanolamines, -glycerols and -serines, where the head group is attached to the third carbon atom in the glycerol backbone. One important feature common to all these lipids was that the glycerol moiety is oriented almost perpendicular to the bilayer surface, with the sn-1 chain continuing in this direction whereas the sn-2 chain starts first in a direction parallel to the layer and then bends sharply at the second carbon atom. This was confirmed by observing a distinct pattern of quadrupole splittings in DMR experiments for the first deuterated methylene segment in both chains. These segments were subsequently found to be out of step by up to three carbon-carbon bond lengths in the neutron diffraction profiles. Here we present neutron diffraction results as well as DMR signals on 2-sn-phosphatidylcholine ( $\beta$ -lecithins) where the head group is attached at the second carbon atom in the glycerol part, such that a symmetric chemical bond pattern arises for the region of the chain attachment. The neutron density profiles as well as the quadrupole splittings from DMR experiments clearly show that both fatty acyl chains have the same conformation. This result indicates that in phospholipids the conformation of the chains near the glycerol backbone is determined by a low intramolecular energy minimum.

**02.6-04** MOLECULAR CONFORMATION OF DIMYRISTOYL LECITHIN (DIHYDRATE). By R. H. Pearson, Biophysics Dept., Roswell Park Mem. Inst., Buffalo, NY, USA, 14263.

The dihydrate crystallizes in platelets with unit cell parameters of:  $a=8.72$ ,  $b=8.92$ ,  $c=55.4 \text{ \AA}$  and  $\beta=97.4^\circ$ . The molecular structure at  $R=17\%$ , based on reflections collected to  $2\theta=80^\circ$ , has been published. (R. Pearson & I. Pascher, NATURE 281,p499(1979)). This structure is stabilized by two orthogonal helices of hydrogen bonded water lying in the plane of the bilayer. The complete structure, based on new data extending to the limit of the copper sphere, will be reported and compared with structures of other phospholipids and other hydration states of lecithin.

**02.6-05** LOW RESOLUTION X-RAY STRUCTURAL STUDY OF LECITHIN BILAYERS WITH INCORPORATED AROMATIC HYDROCARBONS. Iris L. Torriani\* and Rita Z. dos Santos. Instituto de Física, Universidade Estadual de Campinas, Cidade Universitária, 13100 Campinas, São Paulo, Brazil.

High-angle X-ray diffraction diagrams obtained from hydrated dipalmitoyl lecithin (DPL) multilayers showed changes in the diffraction ring from the acyl chains upon introduction of polycyclic aromatic hydrocarbons. Low-angle patterns were obtained for the systems DPL, DPL-Pyrene, DPL-1,2,5,6 Dibenanthracene and DPL-3,4 Benzpyrene. These patterns were subsequently analyzed using the intensities of the lamellar reflections. The electron density distribution normal to the plane of the bilayer was calculated by Fourier synthesis, with a resolution of 7.5 Å. In the case of Pyrene, the electron density map shows a perturbation of the structure in the hydrophobic region, close to the glycerol group. This is in agreement with NMR experiments reported by Vanderkooi et al. (J.Chem.Phys. 63, 3662, 1975). 1,2,5,6 Dibenanthracene incorporation into the bilayers seems to greatly affect the chain packing all along the acyl chains, including the center of the hydrocarbon core region. Calculations are being completed for the DPL-3,4 Benzpyrene system.

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