Some Symmetry Considerations in the One-Dimensional Myelin Lattice

Dear Sir:

Akers and Parsons (1970) claim that (+++++) are the phases of the five main X-ray diffraction maxima observed from the myelin membrane of normal frog sciatic nerves. They experimentally observed the changes in intensity of the individual reflections as a function of uptake of small amounts of heavy metal label. They then attempted to localize the heavy metal label which they "titrated" into the myelin by a computer-analogue technique. Unfortunately the results of their computer-analogue calculations appear to be erroneous. Their results are not consistent with the crystallographic rules of lattice symmetry.

A one-dimensional centrosymmetric lattice was assumed. The lattice has two crystallographically distinct centers of symmetry. Either may serve as the lattice origin. As a consequence only 16 of the 32 possible phase assignments to be considered in the case of the 5 myelin reflections are unique. The other 16 are related to the first ones by choosing the alternate origin.

The theoretical structure factor relative to origin a is

$$F_a(h) = \sum_{j=1}^{N/2} f_j \cos (2\pi h x_j)$$

for a symmetric lattice, where N is the total number of atoms within the unit cell, f_j are the atomic scattering factors for the different kinds of atoms, and x_j are the fractional atomic positional coordinates for the atoms within an assymmetric part of the unit cell. To make the transformation from one origin to the other, $(x_j + \frac{1}{2})$ is substituted for x_j. Since $\cos (2\pi h[x_j + \frac{1}{2}]) = \cos (2\pi h x_j) \cos (h\pi) - \sin (2\pi h x_j) \sin (h\pi)$, the structure factor relative to origin b is

$$F_b(h) = \sum_{j=1}^{N/2} f_j \cos (2\pi h x_j) \cos (h\pi).$$

Thus $F_b(h) = (-1)^h F_a(h)$. Equivalent phase sets are those pairs having identical even-order phases but having sign-reversed odd-order phases.

The general crystallographic question of how phases may be assigned has been studied by a number of workers (Hauptmann and Karle, 1959; Stout and Jensen, 1968). In dealing with a centrosymmetric lattice, it is necessary to place the origin at a center of symmetry. A change of origin from one center to another will affect only the phases and not the magnitudes of any structure factor, hence either origin may be used. A shift of origin results in a change of sign for all reflections of odd h but no changes in $|F(h)|$. Since the phases of the

even h reflections never change, it is clear that they are fixed by the structure (structure invariants) and cannot be given a sign value at will. One odd h reflection can be assigned a phase arbitrarily. The phases of all of the other odd h reflections are now fixed and no further arbitrary choice can be made.

This means that if $(+++++)$ is a solution to the myelin phase problem then $(-+-+-)$ is also a solution. In terms of the Geren (1954) wrapping model for myelin, the crystallographic origin can be chosen either at the center of symmetry between the extracellular protein layers or at the center of symmetry between the cytoplasmic protein layers. One cannot a priori distinguish between them.

Akers and Parsons do not state that $(-+-+-)$ is an acceptable solution to the myelin problem, but by omission from their Table I seem to imply that it is worse than the 15 phase sets selected for inclusion. They further define an R factor which is presumably a measure of acceptability of fit in their computer-analogue studies of heavy atom labeling. They report R values for six pairs of equivalent phase sets. For example, $R(-++++) = 52$ while $R(+-+-+) = 19$ and $R(++-++) = 13$ while $R(-+++-) = 55$. These disparities cast serious doubt upon the validity of their computer-analogue procedures and their phase solution. The rule of crystallographic pair equivalences demands that if a heavy label site is found at $x = 0.0$ and, for example, $R(++-+-) = 13$, then $R(-+++-)$ must $= 13$ for the label at $x = 0.5$.

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Reply to "Some Symmetry Considerations in the One-Dimensional Myelin Lattice" by Albert Hybl

Dear Sir:

We reported our phase sequence, as did previous workers (Finean, 1962; Finean and Burge, 1963; Moody, 1963; Burge and Draper, 1965; Worthington and Blaurock, 1968), only in relation to one of the two possible centers of symmetry of the double membrane repeat unit. While at the present time, a center of symmetry cannot be identified with either mem-