



FIGURE 4 Neutron pair correlation function $d(r)$ of water contained in activated carbon, at room temperature, shown by solid lines for 200% (curve a), 42% (curve b) and 25% hydration (curve c). For comparison, $d(r)$ of bulk water at the same temperature is also drawn (curve d) (43). The dotted lines show the result of a smoothing of the experimental data before Fourier transformation. This demonstrates that the additive oscillations, which appear between 3 and 6 Å, have a physical meaning in contrast with those seen at higher r values.

investigated by X-ray scattering (54); the distortion seen at the level of the second nearest neighbors has been attributed to the bending of hydrogen bonds.

The amount of information about protein-water correlations is small. For neutron diffraction, deuterated samples are required and difficult to obtain. However, the first results have been obtained in the case of a photosynthetic C-phycoerythrin protein for which the X-ray crystallographic structure is known to a resolution of 1.66 Å (55).

C-phycoerythrin is abundant in blue-green algae. Nearly 99% deuterated samples of this phycobiliprotein were isolated from the cyanobacteria, which were grown in perdeuterated cultures (56) (99% pure D₂O) at Argonne National Laboratory. This process yielded deuterated C-phycoerythrin proteins (d-CPE) that had virtually all the ¹H-C bonds replaced by ²H-C bonds. One can obtain a lyophilized sample that is similar to amorphous solids as determined by neutron diffraction (53). As it has been defined in previous works (57–59), the level of hydration $h = 0.5$ corresponds to 100% hydration of C-phycoerythrin which leads to a coverage of about 1.5 monolayers of water molecules on the surface of the protein (60).

The water (D₂O)-protein correlations at the surface of a fully deuterated amorphous protein C-phycoerythrin have been studied by neutron diffraction as a function of both temperature and hydration level (53). The correlation distance of 3.5 Å measured in these diffraction experiments compares well with computer