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Flexibility in protein structure

Although protein molecules have well-defined three-dimensional structures, they are known to have considerable conformational flexibility. This flexibility is not usually distributed uniformly in the threedimensional structure. It is of considerable interest to delineate the relatively rigid and flexible regions in protein molecules. A related problem is concerned with protein hydration. High-resolution X-ray crystallographic studies appear to indicate that a substantial part of the hydration shell is invariant with respect to environmental effects and species variation. The invariant water molecules in the shell are presumably important in the structure and action of the concerned protein. Madhusudhan and Vijayan address these related problems through an approach involving primarily the results of water-mediated transformations (page 165). These reversible transformations, which occur in many protein crystals typically in the relative humidity range 90-93%, are caused by the systematic variation of environmental humidity. When the relative humidity around the native crystal is reduced below a critical value, a quantum of water escapes from the solvent regions in the crystal, which results in abrupt changes in unit cell dimensions, diffraction pattern and solvent content. Vijayan's group has

earlier shown that such transformations provide a useful handle for exploring the variability in protein hydration and its structural consequences. Now Madhusudhan and Vijayan report studies on lowhumidity monoclinic and tetragonal lysozyme, two native crystal forms, and a high-pressure form, which represent a variety of environmental conditions, and delineate the relatively rigid, moderately flexible and highly flexible regions in the lysozyme molecule. Further, 30 invariant water molecules in the hydration shell of the protein have also been identified. Some of these water molecules are involved in stabilizing protein structure while some others appear to have a functional role.

Source of error

A few years ago Emil Wolf showed theoretically that the spectrum of a light source can change on propagation, even in free space, if fluctuations within the source are correlated in certain ways. Wolf also showed that if the optical field at the source obeys a certain law (also derived by Wolf), the spectrum of the source is invariant on propagation. The spectral changes that Wolf showed include frequency-dependent redshifts and blueshifts of spectral lines and line broadening. This means that the spectrum of a light source that shows correlation properties, when recorded at a great distance from the source, can show line shifts independent of source movement. This has very important implications in astronomy and astrophysics. Wolf's model of spectral change due to source correlation (also shown experimentally) has a bearing on the long-standing 'redshift controversy' in astronomy. The controversy concerns the large redshifts of some astronomical objects, particularly quasars, and has to do with the difficulties that large redshifts pose for the currently held cosmological theory. The sourcecorrelation model provides a basis for a non-cosmological component of redshift in spectra of astronomical sources. In addition, quasar spectra have peculiar features, including small differences in redshift values of different spectral lines; the sourcecorrelation model also predicts a frequency dependence of line shifts. An article by H. C. Kandpal et al. (page 152) discusses Wolf's theory, the experimental evidence, and implications for spectroradiometric measurements. The authors show that, if spectral shifts due to source correlation are not accounted for, they introduce errors in spectroradiometric measurements. Further, comparisons of spectroin radiometric scales maintained by standards laboratories, sourcecorrelation effects due to differences between optical set-ups become important.