ML. 17–H 2 DNA-PROTEIN RECOGNITION. By B.W. Matthews, Institute of Molecular Biology and Department of Physics, University of Oregon, Eugene, Oregon 97403.

The structures of three proteins that regulate gene expression have been determined recently in different laboratories and suggest how these proteins may bind to their specific recognition sites on the DNA (Takeda et al. Science (1983) 221, 1020-1026). One protein (Cro) is a repressor of gene expression, the second (CAP) usually stimulates gene expression and the third (λ repressor) can act as either a repressor or activator. The three proteins contain a substructure consisting of two consecutive α-helices that is virtually identical in each case. Structural and amino acid sequence comparisons suggest that this bihelical fold occurs in a number of proteins that regulate gene expression. DNA-protein recognition appears to be based primarily on a network of hydrogen bonds as well as other interactions between side-chains of the protein and the parts of the base-pairs exposed within the major groove of the DNA.

It appears that the DNA maintains a right-handed Watson-Crick B-form when either Cro, CAP or λ repressor is bound, although some bending or other deformation may occur.

As well as describing the above structural studies the talk will also review very recent developments in the field including the determination of the structure of the complex of the restriction enzyme EcoR1 with DNA by J. Rosenberg and coworkers, and the structure of a DNA binding protein from Bacillus stearothermophilus by I. Tanaka and colleagues.

ML. 17–H 4 X- AND GAMMA-RAY LASERS AND ADVANCES OF NON-LINEAR X-RAY OPTICS IN CRYSTALLOGRAPHY. By Runar N. Kuz'min, MGU, Physic. Fac., Leninskie Gory, 117234 Moscow, USSR.

The future of structure analysis and X-ray optics depends on new types of sources of powerful coherent electromagnetic radiations with wave length near 1 Å. At present, the scientists in many countries initiate studying this problem. Therefore, a review about the theoretical and experimental results in this new field of physics is of great interest for the Crystallography Congress. Furthermore, this subject is not treated in any other report.
Contents: 1. X-ray and gamma-ray lasers, 2. coherent radiation of nonlaser powerful sources, 3. electrodynamics lasers, 4. nonlinear X-ray optics, 5. inelastic scattering, 6. coherent effects in inelastic scattering, 7. collective states, 8. applications in structure crystallography.
Theoretical and experimental investigations in the field of development of X-ray lasers is described; lasers based on free-electron beams, lasers based on the inverse Compton effect, Vavilov-Cerenkov radiation, coherent bremsstrahlung, transition radiation, coherent positron and electron channelling radiations, incoherent Coulomb excitation, and crystal undulators will be discussed. The review treats the following forms of linear spontaneous inelastic X-ray scattering: coherent Compton and Raman effects, plasmon and parametric scattering. The problem of nonlinear interaction of waves in a material and the theory of collective spontaneous emission of X- and γ-rays in periodic structures are treated. Some applications to X-ray diffraction analysis are described.

Zh.Tekh.Fiz., 44, 194; 2568 (1974); Usp. fiz. nauk, 114, 677 (1974); 120, 82 (1977); 126, 479 (1978); Pisma v ZhETF, 29, 30 (1979); 34 248 (1981); ZhETF, 83, 878 (1983);Fiz. Tverd. Tela, 24, 3718 (1982); Mössbauer Spectrocopy, ed. by U. Gonser, p. 49, (1981).

ML. 18–H 2 The Study of Macromolecular Interactions by Computer Graphics. By Arthur J. Olson, Member, Department of Molecular Biology, Research Institute of Scripps Clinic, 10666 N. Torrey Pines Road, La Jolla, California, 92037.

A deep understanding of the function of biological macromolecules and their assemblies is coming from analysis of the three dimensional atomic resolution structure of these systems. Computation and computer graphic analysis is playing a pivitol role in such studies. Real time interactive display of protein and nucleic acid structures is now available in roughly 100 laboratories throughout the world. Such facilities are being used to aid in the process of x-ray crystal structure determination and in the analysis of the resulting three dimensional structures.

The past few years have seen an increasing application of computer graphics to the understanding of macromolecular interactions. Focus has been placed upon the calculation and display of properties relevant to these interactions. The solvent accessible molecular surface as defined by Richards (Annu. Rev. Biophys. Bioeng. (1977) 6, 151), and implemented by Connolly (Science (1983) 221), provides an analytical basis for examining surface topography and the steric factors that influence macromolecular interactions. Mapping electrostatic characteristics onto this surface (Kollman, et al, Nature (1983) 306), and extending the electrostatic analysis to include the three dimensional field surrounding the interacting species (Getzoff, et al, Nature (1983) 306), enables examination of influences at a distance.

This lecture will discuss the development and application of computer graphics to the analysis of interacting macromolecular systems, including the study of assembled supramolecular systems and the modeling of macromolecular docking. A computer animated film illustrating this work will be shown.