02.4-03 CRYSTALLOGRAPHIC STUDIES OF METAL BINDING TO TRANSFER RNA. By J. R. Rubin and M. Sundaralingam, Department of Biochemistry, College of Agricultural & Life Sciences, University of Wisconsin-Madison, Madison, WI 53706

The role of cooperatively bound cations in the stabilization of biologically active conformers of tRNA is well established. Previous crystallographic studies on the magnesium form of phenylalanine tRNA from yeast have shown the presence of three to four tightly bound magnesium ions located in the tertiary structural folds of the molecule. As a continuation of our structural studies on tRNA and its interactions with biologically important ligands (Liebman et al., Proc. Natl. Acad. Sci. USA, 72, 4821 (1977)), we have now examined the binding of a series of transition metal ions and complexes to crystalline phenylalanine tRNA by x-ray crystallography.

Zinc salts have been shown to substitute for magnesium in the enzymatic aminoacylation of tRNA. A crystalline complex of Zn(II)-phe tRNA prepared by soaking native phe tRNA crystals in $ZnCl_2$ solutions shows at least five strong binding sites for zinc on the molecule. The two major zinc binding sites correspond to magnesium binding sites in the structure. All but one of the zinc binding sites involves direct coordination to N7 of guanine bases, including G20, G15, G65 and G43. Similar studies on the binding of other metals e.g. Cd^{++}, Pb^{++}, Ni^{++}, Cu^{++} etc. are in progress. The effects of such metal ion binding on the conformations of tRNA will be discussed.

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02.4-04 POLYMORPHISM IN DNA-RNA HYBRIDS. By Struther Arnott, R. Chandrasekaran, A. Banerjee, A.G.W. Leslie and E. C. Selsing, Department of Biological Sciences, Purdue University, West Lafayette, IN 47907, U.S.A.

DNA-DNA duplexes are quite polymorphic with a range of helical structures in which the average axial translation per nucleotide $0.26\ nm \leq h \leq 0.38\ nm$ and the corresponding rotation $-30.0° \leq t \leq 48.0°$ are both quite variable (Leslie *et al*, J. Mol. Biol. (1980), 143, 49-72; Arnott, Biophys. J. (1980) 32, 249-250). RNA-RNA helical duplexes are much less variable: all known allomorphs have qualitatively similar conformations although $0.26\ nm \leq h \leq 0.31\ nm$, $30.0° \leq t \leq 32.7°$. Our systematic fiber diffraction analyses of poly dN.poly rN' (where N = A, T or U, G or I, C and N' = the Watson-Crick complement of N) have revealed that in general DNA-RNA hybrids are isomorphous with *A*-DNA (Fuller *et al*, J. Mol. Biol. (1965), 12, 60-80) in less hydrophilic environments, but isomorphous with *A'*-RNA (Arnott *et al*, Nature (1968), 220, 561-4) in more hydrophilic environments. In addition an unique duplex allomorph (h = 0.32 nm, t = 36.0°) observed with poly dI·poly rC may have the hitherto unobserved conformation which was mistakenly proposed for *B*-DNA by Crick and Watson (Proc. Royal. Soc. A (1954), 223, 80-96).

02.5-01 CRYSTALLOGRAPHIC ANALYSIS OF EcoRI ENDONUCLEASE-DNA COMPLEX. By John M. Rosenberg, John Grable, and Christin Frederick, Dept. of Biological Sciences, Univ. of Pittsburgh, Pittsburgh, PA 15260; Patricia Greene, Dept. of Biochemistry, Univ. of Calif., San Francisco, CA 94143; Keiichi Itakura, City of Hope Medical Center, Duarte, CA 91010; Horace Drew, Dept. of Chemistry CalTech., Pasadena, CA 91125; and Roberto Crea, Genentech, So. San Francisco, CA 94080.

A recognition complex between EcoRI endonuclease and a synthetic oligonucleotide (sequence CGCGAATTCGCG) crystallizes in space group P321 with unit cell parameters a = 128 Å and c = 47.3 Å. The presence of the DNA was confirmed by single crystal ultraviolet microbeam spectroscopy. The most likely asymmetric unit contents are one 31,000 dalton enzyme subunit and one strand of DNA, yielding a V_M of 3.11. This implies that the DNA-protein complex obeys two-fold rotational symmetry, which has been incorporated in the crystalline lattice. Large monoclinic crystals have also been obtained in the absence of DNA; their space group is C2 with a = 211 Å, b = 128 Å, c = 49 Å, and β = 98.5°. Striking similarities between the lattices and diffraction patterns of these two forms have been noted. Structure analysis is in progress. Supported in part by NIH grants No. GM-25671, RR-07084 (JMR) and GM-25729 (PG).

02.5-02 STRUCTURE OF THE BACTERIOPHAGE LAMBDA CRO REPRESSOR: MODEL FOR PROTEIN-DNA INTERACTIONS. by W.F. Anderson*, D.H. Ohlendorf†, Y. Takeda‡, B.W. Matthews†. *Department of Biochemistry, University of Alberta, Edmonton, Alberta, T6G 2H7, Canada. †Institute of Molecular Biology, University of Oregon, Eugene, Oregon, 97403, U.S.A. ‡Chemistry Department, University of Maryland, Baltimore County, Catonsville, Maryland, 21229, U.S.A.

The bacteriophage lambda cro protein is a small (66 amino acids) polypeptide which binds to specific DNA base sequences in the lambda genome. We will present the three-dimensional structure of the cro repressor and its apparent mode of interaction with operator DNA. The postulated interaction between repressor and operator is consistent with a variety of chemical and genetic evidence, and may provide a general model for the interaction of proteins with helical DNA.

A principal feature of the proposed binding of cro to DNA is the use of symmetry. The two-fold symmetry axis of the repressor coincides with the approximate two-fold symmetry axis of the DNA operator. This type of interaction is expected to be of general significance for proteins which recognize symmetric, sequence-specific regions of the DNA. Our results indicate that the symmetric sequences often used for specific DNA-protein interactions are a consequence of the oligomeric structure of the regulatory proteins rather than the source of special type of DNA structure.

The proposed model places two-fold related α-helices in successive major grooves of right-handed B-DNA. The amino acid side chains extending from this helix would then provide the base sequence specifity of the cro repressor operator complex. Evidence for a similar structure in some other DNA binding proteins will be presented.