02.4–3 CRYSTALLOGRAPHIC STUDY OF THE COMPLEX BETWEEN THE Fab FRAGMENT OF MONOCLONAL ANTI-LYSOZYME ANTIBODY AND ITS ANTIGEN. By A.G. Amit, G. Boulot, M. Harper, D. Jankovic, A. Le Guern, R.A. Mariuzza, J.C. Mazié, S.E.V. Phillips and R.J. Poljak, Institut Pasteur Département d'Immunologie, 75724 Paris, France.

Current understanding of the structure of antibody combining sites is based on the three-dimensional structures of the Fab fragments of myeloma proteins and their complexes with small molecules. No crystallographic information is available for the interaction of an antibody with a macromolecular antigen, however, even though such interactions are more extensive and potentially more important for the elucidation of the physiological properties of antibodies. We have used the lymphocyte fusion techniques of Köhler & Milstein to obtain hybrid cell lines secreting monoclonal anti-hen eggwhite lysozyme (HEL) antibodies. Complexes between the Fab fragments of several of these antibodies and HEL were prepared and subjected to crystallization trials. One of these complexes (Fab D1.3-HEL) was crystallized from PEG solutions in space group $P2_1$ with a= 55.7 b= 143.5 c= 49.1 β = 120.5°. Rotation photographs show reflections to at least 2.0 Å resolution using synchrotron radiation (Mariuzza et al.1983 J. Mol. Biol. 170, 1055-1058).
Diffractometer data have been collected to 6 Å resolution for a native crystal and three derivatives. The derivatives were solved from isomorphous difference Patterson maps, and refined using the F_{hle} method. Phase calculation gave a mean figure of merit of 0.75. The electron density map clearly shows the molecular boundaries, and the immunoglobulin domains are recognizable. There is no clear boundary between the densities corresponding to the Fab fragment and lysozyme, indicating a close intermolecular interaction.

02.5–1 STRUCTURE OF SINGLE-STRANDED POLY (2'-O-ETHYLCYTIDYLIC ACID)—THE EFFECT OF ALKYLATION ON POLY (C).

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2'-O-alkylated polynucleotides are of considerable biological interest, in view of the presence of 2'-O-methyl nucleotide residues in tRNA, rRNA, mammalian and viral mRNA; and of 2'-O-ethyl nucleotide residues in liver tRNA following L-ethionine induced hepatic carcinoma[1] in the rat. There is a speculation that 2'-O-alkylation might be responsible directly or indirectly for the irregularities[2] in the backbone conformations of the polynucleotides.

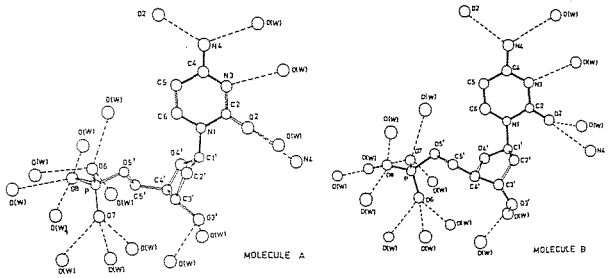
X-ray diffraction of poly (2'-O-Ethylcytidylic acid) in polycrystalline, moderately oriented fibers at pH 6.8 adopt a 6-fold helical structure (single stranded) with an axial rise per residue of 0.315 nm, very similar to poly(C)[3] and poly(Cm)[4]. The form observed at 66% RH has orthorhombic ($P2_12_12_1$) symmetry and cell dimensions a=1.65 nm, b=2.19 nm, and c=1.89 nm. Close similarity of diffraction pattern and cell dimensions of poly (Ce) and poly (Cm) along with the present structural study strongly suggests that (a) alkylation at O2' does not change the C_3 endo pucker of the furanose ring and (b) the prerequisite to six fold helical structure is not necessarily the intermolecular hydroxyl-hydroxyl hydrogen bonds as evidenced in poly(C) rhombohedral crystal structure.

Reference: 1) Kielanowska, M. and Sugar, D. (1976), Nucleic acid Res, 3, 817-823; 2) Cheng, D.M. and Sharma, R.H. (1977), Biopolymer 16, 1687-1711; 3) Leslie, A., Chandrasekharan, R, Arnott, S. (1976), J.M. Biol, 106, 735-748; 4) Leslie, A. and Arnott, S. (1978), J.M. Biol, 119, 399-414.

02.5–2 STRUCTURE OF DEOXYCYTIDINE 5'-PHOSPHATE 5'-dCMPNa$_2$.11H$_2$O By J.Pandit, T.P.Seshadri and M.A. Viswamitra, Department of Physics and ICMR Centre on Genetics and Cell Biology, Indian Institute of Science, Bangalore 560 012, India.

Interactions with cations and water molecules are expected to play an important role in influencing nucleotide conformations. We report here the structure of a highly hydrated form of 5'-dCMP. A striking feature of the structure is that the two independent molecules in the crystal have *identical environments but totally different nucleotide conformations*. (see Figure below)

Crystal data are: P1,
a = 7.306(2), b = 10.055(2), c = 16.670(2) Å
α = 101.93(1)°, β = 93.07(1)°, γ = 90.89(2)°, Z = 2,
R = 0.065. Molecular conformations are Molecule A: anti (χ = 231.7°) C2'-endo, gauche-gauche; Molecule B: anti (χ = 195.3°), C3'-exo, gauche-trans.



A pseudo-inversion symmetry is present in the crystal, which applies to all the solvent and molecular atoms except for the atoms on the furanose ring. The interactions between the nucleotide and water/sodium ions are exactly identical in the two molecules as a consequence of this symmetry. The presence of such a partial enantiomorphic relationship between the two molecules suggests the interesting possibility that these molecules could serve as the *monomer units for generating left and right handed DNA structures*.

Another noteworthy feature of the molecular interactions is the pronounced stacking of the cytosine rings (see Figure below) a feature also present in the orthorhombic crystal form of the same nucleotide (dCMP.Na$_2$.7H$_2$O, Pandit, Seshadri and Viswamitra (1983), Acta Cryst. C39 342). Modelling studies with the bases stacked as in the crystal structures show the possibility of a *self intercalating double helical model for poly (dC)* (Viswamitra and Pandit (1983), J.Biomol. Struct. & Dynam. 1 743).