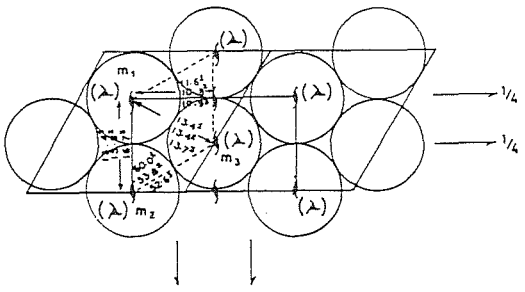
02.5-5 VISUALISATION OF RELATIONSHIP OF SYMMETRY, CONFORMATION IN BIOLOGICAL MACROMOLECULAR STRUCTURE AND FUNCTION - A TYPICAL CASE OF POLY(C) AND ITS ANALOGS. By A.C. Gomes, G. Biswas, R. Lalwani, S. Chakraborty, K. Bera and A. Banerjee. Biophysics Department, Bose Institute, Calcutta-54, India.

Implications of structural symmetry, conformation, order, disorder in macromolecular assembly is discussed to clarify "fuzziness" in relation between structures and biological functions. Experimental study and modelling reveals that like B-DNA, in semicrystalline matrix, the molecular internal symmetry is nicely exploited in the poly(C) and its analogs, poly (Cm) and poly (Ce) in the molecular assembly pattern. In macromolecular assembly and self organization, the internal symmetry (if any) of the molecule is usually involved for biological functions via proton transfer efficiency and involves hydrogen bonding. In the present study, the basic monomer units of poly(C), poly(Cm) and poly(Ce) are same, except the modification of 2'-0 position of furanose ring in cytidylic acid. X-ray fiber diffraction and modelling studies of all three above polymer adopt a 6-fold helical structure at 6.8 pH and 66% relative humidity. It is noteworthy that poly(C) and its analog structures stack like pile of pennies each rotated by 60^{o} relative to each other in a right hand screw. The extent of perturbation and steric pressure produced by the modification at 2'-0 position is absorbed by the system in the long range structure. This has been possible due to special position that is adopted by the modified group as a side pendent to the helical structure with a minimum steric pressure. Poly(C) has exploited the internal molecular 6_1 symmetry where as in poly(Cm) and poly(Ce) the hydroxyl group of 2'-0 position are blocked by CH_3 and C_2H_5 groups and make unfavourable for hydrogen bonding and the system radily record that by lowering the system symmetry to 2_1. In poly(C), the three neighbouring molecules sitting at 3-fold screw axis with an angle 60^{o} observed from experimental cell parameters. But in the case of poly(Cm) & poly(Ce) the angles are 53.8^{o} & 52.6^{o} observed from experimental data. The occurance of this 60^{o} angle depends on the symmetry of the poly(C) molecule and on the favourable disposition of intermolecular contacts. This argument justifies the augmentation of the lattice convolution over the molecular transform and naturally, poly(C) offers a good discreate rotation diffraction diagram as expected. This may be the fact that more the departure from the angle 60^{o} in packing arrangement, more would be strain or release of strain of the favourable contacts providing less favourable lattice convolution, hence less discrete spots in the diffraction pattern as expected in the case of poly(Cm) and poly(Ce). Hence the lattice symmetry and unit cell parameters are influenced as when necessary induced by the internal symmetry of the molecule to adopt a most favourable lattice disposition of the molecule under given situation. Trivial deductions shows nearest neighbour molecular distances center to center are 13.4 Å, 13.4 Å for poly(C);13.4 Å, 15.8 Å for poly(Cm) and 13.7 Å and 16.7 Å for poly (Ce).



Assembly (packing) pattern of poly(C)[1], poly(Cm)[2], poly(Ce)[3].

02.5-6 TRANSITION TOPOLOGY OF GENE STRUCTURE - A GENERALISED DNA MODEL WITH DUAL ROLE IN DNA PHASE TRANSITION. By R. Lalwani, S. Chakraborty and Asok Banerjee, Biophysics Department, Bose Institute, Calcutta 700 054, India.

The topological problem in the DNA double helix, the high linking number ($3x10^5$), the existence of different structural units, and the different Tm values for isocompositional but different sequences all indicate a need for a fresh look at the DNA paradigm. Insertion of stretches of AT or TA pairs within GC shows that syn-anti alternation is the necessary and sufficient condition for Z-DNA formation, which is heading to a partial (guanine preference) random sequence. We arrive at two attractive models: (a) All-syn nucleotide, W-C base paired but with chain reversed to conventional B-DNA (minor groove view). This model switches left to right favourably in a continuous way in which dynamic inversion of sugar moiety (C3 endo ⇋ C2 endo) and (3'-5') direction are dominant factors. (b) All-anti classical B-DNA. B-Z transition is visualised only via strand exchange, hydrogen bond break and reanneal. In our view both all-anti and all-syn W-C type DNA double helices are realities and take part in DNA phase transition. Intermediate forms are a mixture of DNA chains having antiparallel (i) right handed helices, (ii) left handed helices, (iii) one right and one left handed helix. Antiparallel chains and complementary base pairing are the necessary conditions for DNA replication which both the competing models satisfy, the basic criteria demanded in molecular biology. It is hard to reject either of the two. The reversal in chain direction in the two models is also observed in B and Z-DNA structures (X-ray data) with distinct differences in major and minor groove size.

Our generalised model is a single DNA polymeric chain with nucleotide as repeat unit. The complex between such polymeric antiparallel chains with W-C base pairing forms DNA double helix. The all-anti chain direction is reversed in all-syn model to maintain favourable W-C pairing. The probability of double helix formation of either is 1/2. There is evidence that both right and left handed DNA forms coexist in dynamic state in vivo. The preference of either will come naturally from environment/sequence/composition and/or inducing enzyme via dynamic strand association, dissociation and breathing phenomena of DNA. The principle of protein DNA interaction via proton transfer efficiency at organization is operative in DNA double helix complex too.

This model distinguishes itself from conventional ones and points to the dual role of DNA in right ⇋ left transition and necessity of syn ⇋ anti conversion for base pair preservation.