adenines. The bases in the base pairs are not in a plane and are bent about the center of the duplex forming a pleat. A3 and A6 which swing out are within stacking distances but have only limited partial stacking. A water molecule OW2 hydrogen bonded to N(7) of A1 is stacked on top of A6 forming a half-sandwich (R. Parthasarathy, T. Srikrishnan & S.L. Ginell in Biomolecular Stereodynamics, R.H. Sarma, Ed. Adenine, New York, 1983). On the other hand, the base A3 of the dimer is not involved in such a stacking interaction with a water molecule since N(7) of A4 is hydrogen bonded to a neighboring A1 and not to any water molecule. Crystals of II are tetragonal, $P4_1$ with cell constants a = b = 14.070(1), c = 43.906(5)Å, Dobsd. = 1.56 g.cm^{-3} for $(C_{30}H_{37}N_{15}O_{16}P_2)_2$. 11 H_2O. Using complete three-dimensional intensity data to the limit of Cu sphere (10077 reflections, 7044>3σ), the structure was solved using MULTAN 80 and weighted Fourier syntheses to an R-value of 0.064. All the six adenosines show anti conformation across the glycosidic bond and a range of puckers of the C3'-endo family. The two helical segments A1+pA2 and A4pA5+ show the preferred (g^-, g^-) conformation whereas the non-helical loop segments A2pA3$^+$ and A5$^+$pA6$^+$ show (g^+, g^+) conformation. The agreement index $R_{symm.}$ between hkl and khl for form II is 0.38 indicating the lack of crystallographic two fold axis. We also have collected data from other crystals for which $R_{symm.}$ had values of 0.08, 0.12 and 0.32. Work is in progress on these crystals. Work supported in part by NIH GM 24864.

02.5-3 THE Z-DNA COMPATIBLE SEQUENCE d(GTGTACAC) CRYSTALLIZES AS A-DNA.

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The molecular structure of a self complemetary DNA octamer, GTGTACAC has been solved to 2.5 A resolution using single crystal x-ray diffraction methods. The cell constants of the crystal are, a=42.43 A, c=24.15 A, space-group, $p4_32_12$, Z=4 (duplexes). The molecule forms a right-handed A-DNA-like double-helical structure with characteristic shallow and deep grooves, but does not have the typical base-pair tilt of A-DNA. Currently the residual R-factor for the reflections out to 2.5 A is 24.5% and the waters of hydration have still not been included. Further refinement of the structure is in progress.

The results are of much interest since (GT)n/(CA)n sequences are widely distributed in natural DNA (E.N. Trifonov, et.al., 1985, FEBS 185, 197). Moreover, the GTG/CAC triplet occurs very frequently in genomic regulatory regions, and also has some unusual physical properties (P. Lu, et.al., 1983, J. Biomolec. Struc. Dyn. 1, 509). Some investigators have suggested that these sequences may be involved in formation of the left-handed Z-DNA structure (A. Nordheim, A. Rich., 1983, Proc. Nat. Acad. Sci. USA 80, 1821), but in-vivo experiments have yielded no evidence in favor of this hypothesis (A. Rodriguez-Campos, et.al., 1986, EMBO 5, 1727; D.S. Gross, et.al., 1985, J. Mol. Biol. 183, 251). Our results also demonstrate that such a sequence adopts a right-handed rather than a left-handed conformation.

02.5-4 NUCLEIC ACID JUNCTIONS AND MACROMOLECULAR DESIGN. By N.C. Seeman, C.J. Newton, M.L. Petrillo, J.-H. Chen, J.E. Mueller, J.A. Maiorella, and R.D. Sheardy, Department of Biology, SUNY/Albany, Albany, NY 12222; R.-I. Ma and N.R. Kallenbach, Dept. of Biology, University of Pennsylvania, Philadelphia, PA 19104, USA.

The Watson-Crick base-pairing interactions of nucleic acids constitute a particularly powerful system for controlling the structure and connectivity of these polymers. For many years, molecular biologists have formed specific linear double helical molecules by mixing pairs of complementary single strands. Recently we have shown that stable branched nucleic acid complexes, called junctions, can be formed from mixtures of 3, 4 or 5 oligonucleotide single strands with carefully selected sequences (N.R. Kallenbach, R.-I. Ma and N.C. Seeman, 1983 Nature 305 829-831); these complexes contain multiple double helical arms all coming from a central point. The fundamental rule in implementing the sequence selection algorithm is the minimization of sequence symmetry.

Nucleic acid junctions are analogs of ephemeral intermediates seen in the processes of replication and recombination, and we are exploring the structural, dynamic and thermodynamic properties of these structures from that perspective. From circular dichroism spectroscopy, it is clear that the junction does not perturb the structure of the arms. Nuclear magnetic resonance spectroscopy has indicated that the bases which flank the junction are paired. Combined gel electrophoretic and oligomerization-ligation studies have indicated that a large range of 3-dimensional structures are available to junctions. Crystallization is in progress.

Besides being important objects of study, junctions may be regarded as macromolecular valence clusters with specifically addressable ends, particularly if asymmetric sticky-ended associations are employed. The idea is to construct geometrical figures and N-connected networks, in which the edges are double helical nucleic acids, while the vertices are nucleic acid junctions. Preliminary experiments indicate that hydrogen-bonded base-pairing of cohesive ends can be used to direct the formation of linked clusters as well. It is worth noting that this system is more complicated than simple valence clusters composed of atoms connected by bonds: In this larger system, the twist of the double helices plays an important role in determining the shape of the products. Indeed, changing the number of nucleotide pairs between junctions can alter both the geometry and the topology of an array of junctions. In addition, it appears that the system can respond to torsional stress by altering the structure of the junction itself.

This junction-association system offers a useful paradigm for understanding crystal formation, since the intermolecular contacts are pre-determined: It has prompted the recent suggestion of an entropic driving force to explain the small number of molecules (typically one) seen in the asymmetric units of molecular crystals. In particular, we have put forward the idea that the maximization of entropy in reciprocal space is similar to the expansion of a gas in direct space, $\Delta S = R \ln (\bar{V}_2/\bar{V}_1)$ (N.C. Seeman, 1985 J. Biomol. Str. Dyns. 3, 11-34). The goals of this part of the work also include the rational design of crystals and the fabrication of mechanical and electronic devices on the nanometer scale.

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