adene. 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 GW2 hydrogen bonded to N(7) of A1 is stacked on top of A6 forming a half-sandwich. ita. Kari Pulli, & J.I. Newton, Jr. (1986) Nature 324: 371-374. 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 used specific linear double-helical molecules by mixing pairs of complimentary 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 H.C. Seeman, 1986 Nature 309:829-831); these complexes contain multiple double helices 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 spherical intermediates seen in the process of replication and recombination, and we are exploring the structural, dynamic and thermodynamic properties of these structures from that perspective. From circular dichroism, the preferred (g.g.->g.g.) helices, indicate that base pairing does not perturb the structure of the arms. Nuclear magnetic resonance spectroscopy has indicated that the bases which flank the junction are protected by the solvent. Electrophoretic and oligonucleotide-fragmentation 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 partially crossed 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 clustered composed of atoms connected by bonds: In this larger system, the twist of the double helix plays an important role in determining the shape of the products. Indeed, changing the valence clusters with 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 the polymerization, 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 minimization of entropy in reciprocal space is similar to the expansion of a gas in direct space, $\Omega = R Y_{ij}$ (H.C. Soeman, 1985 J. Biomol. Struct. Dyn. 3:11-24). The goals of this part of the work also include the rational design of cluster and the fabrication of mechanical and electronic devices on the nanometer scale.

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