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Polarized Intercalation Site in Z-DNA

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Z-DNA can support an intercalation conformation exhibiting the 5′-pu-p-py-3′ sequence specificity in contrast to the experimentally observed in B-DNA intercalation X-ray crystallographic DNA: drug models, however the binding site in Z-DNA is determined by the alternating *anti-syn* backbone rather than base sequence. Z-DNA also exhibits a conformationally polarized intercalation site within the dimer repeat unit that is consistent with the neighbor exclusion principle. Additionally, Z-DNA conformers exhibit (positive) winding of the dimer repeat unit upon assumption of the intercalation conformation.

Keywords: Z-DNA, intercalation, conformationally polarized

INTRODUCTION

Z-DNA exists as a left-handed helix with Watson-Crick base pairing and is characterized by alternating *anti-syn* glycosidic bonds. The structure of Z-DNA was first obtained for (5′-G-p-C-3′)$_6$ and analysis of the crystal structure showed that the C base retained the normal *anti* orientation while the G base had switched to the *syn* orientation, resulting in an *anti-syn* dimer as the repeat unit. The bases in the Z-DNA molecule are stacked perpendicular to the helix axis, forming a structure that is more compact than B-DNA with 12 bases per turn of the helix [1, 2]. The exact physiological role of Z-DNA is not known, however recent studies indicate that it may play a role in the editing of RNA during transcription [3].

Conversion of B-DNA to Z-DNA results from the rotation of the base pairs by 180° around their long axis (C1′ to C1′ of the base pair deoxyribose sugars). In poly GC this is accomplished by the rotation of G around the glycosidic bond, resulting in the *syn* conformation, while the entire base pair is rotated in the case of C, allowing preservation of the *anti* conformation [4, 5]. The ability of a particular DNA to switch from the B- to the Z- conformation is dependent on its base sequence, with (5′-G-p-C-3′)$_n$ being the most favorable sequence. However a number of studies have shown that, although alternating purine-p-pyrimidine sequences are most favorable, the base sequence can vary as long as the *anti-syn* conformation is conserved [1, 2, 4, 6–8]. The equilibrium of the B- to Z- transformation is dependent on ionic strength, pH, temperature, pressure, the pre-

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sence of specific ligands, and supercoiling of the DNA [1].

Prior to the introduction of the Z-DNA structure, [4, 9, 10] some of the theoretical and experimental research on DNA during the 1970s and into the 1980s focused on drug: DNA complexes [11–46] Z-DNA is the only DNA structure for which exact coordinates exist in the absence of intercalants. Models of other DNA variants such as A- and B-DNAs arise from X-ray diffraction of fibrous specimens. The intercalation models present X-ray crystallographic data for samples consisting of dimer duplex DNA and a drug, and provide exact coordinates. The intercalation sites of classical B-DNA: drug systems have generally exhibited a pyrimidine-p-purine (5′-py-p-pu-3′) sequence [11–29].

In this investigation the sequence 5′-C-p-G-p-C-p-G-3′ served as the model sequence for Z-DNA. Such a tetramer duplex sequence is the minimum number of base pairs required to characterize the conformational properties of an intercalation site. For B-DNA such a sequence is a fragment of a decamer while for Z-DNA, it is a fragment of the dodecamer.

During the course of examining the conformational domains available to Z-DNA, [47] the base pairs were permitted to assume their maximum separation, which set the stage for elucidating potential intercalation sites in Z-DNA. Since the repeat unit of Z-DNA is a dimer duplex (5′-C-p-G-3′ 5′-G-p-C-3′), a tetramer duplex segment contains two distinctly different backbone parameter regions, one that is *syn-anti* (5′-G-p-C-3′) and the other with an *anti-syn* (5′-C-p-G-3′) conformation [1]. This feature potentially permits Z-DNA to have two different intercalation sites, the *anti-syn* site designated as site 1 (5′-C-p-G-3′), between BP3 and BP4 in Figure 1, and the *syn-anti* site designated as site 2 (5′-G-p-C-3′), between BP2 and BP3 in Figure 1. It should be noted that the potential binding site between BP1 and BP2 is identical to site 1, due to the dimer repeat unit of Z-DNA. A search for the

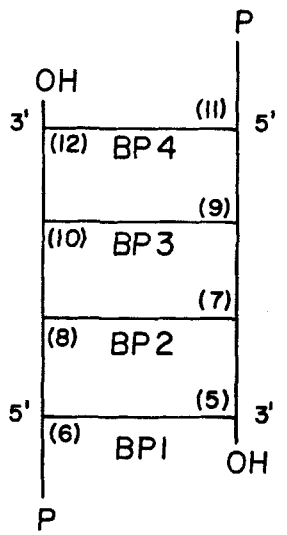

FIGURE 1 Schematic representation of a tetramer duplex DNA. BP1 is base pair 1, and so on to BP4. The deoxyribofuranose sugars and associated phosphate groups of BP1 are denoted by (5) and (6). Similar notation applies for the backbone units of the other three base pairs. The intercalation site (see text) resides between BP2 and BP3.

intercalation sites permitted by the Z-DNA repeat unit reveals that the binding site is conformationally polarized, i.e., only one of the two possible domains can separate enough to allow intercalation. The maximum separation of the base pairs in this domain is 7.0 Å.

This study utilized a desktop computer [48, 49] using a Fortran compiler [50] to run the Generalized Algorithm to Generate Nucleic Acid Structures (GAGNAS) [34]. Graphics utilized a desktop computer version of Dissipla [51] made available on a beta test basis. GAGNAS searches through a number of incremented, defined helical parameters designating the orientation between two adjacent base pairs within a dimer duplex seeking the closure of the sugar-phosphate backbone with experimentally acceptable bond angles and bond lengths. Experimental structural data as well as GAGNAS energy calculations of the resulting dimer duplexes serve as the criteria for selection of the segments that are chained to construct a DNA. The dimer duplexes are then chained together to form a

DNA polymer of any desired length that can then be subjected to a number of changes corresponding to modifications of the DNA.

This work examines the conformationally allowed range of Z-DNA structures permitting intercalation. Such an approach examines Z-DNA in a mathematical sense. Though solvent effects are generally considered, the question of a given conformation available to the Z-DNA is a mathematical matter dependent upon the ability to complete the backbone for a given set of helical parameters defining the DNA. Thus Z-DNA conformation can be examined in a purely mathematical sense as it pertains to appropriate bond angles, bond lengths, glycosyl torsion angles, sugar ring pucker conformation and helical parameters. Although the effect of salt concentration was not taken into account in the calculations, it has previously been shown that with GAGNAS the addition of a counter charge of +1 to the PO^{2-} group on the phosphate backbone results in a change in the total energy of the structure, but the relative energy-dependence of the parameters remains unchanged [29].

PARAMETERS SEARCHED

The helical values of the DNA search ranged as follows [52]: α_z, −10° to −60° by −5°; ΔZ, 3.40 Å to 7.6 Å by 0.2 Å; α_y, 0° and −8°; ΔY = 0.0 Å; ΔX, −3.0 Å to 5.0 Å by +1.0 Å; χ_G, −20.0° to −70.0° by −5.0°; χ_C, 20.0° to 90.0° by 5.0° with the sugar pucker of the *G* base set to C1′-*exo* (C1X) and that of the *C* base set to C2′-*endo* (C2N).

ENERGY FUNCTIONS AND CONVENTIONS

The energy functions consist of the classical 6–12 potential with Suter modification, [53] terms accounting for gauche-gauche effects, lone-pair electron repulsions of the phosphate oxygens, hydrogen bonding, and solvent effects all described elsewhere [32, 40]. Figure 1 schematically illustrates the convention followed to designate the DNA structure in the GAGNAS. The base pairs, numbered BP1 to BP4 comprise a tetramer duplex. Each of the associated sugar-phosphate fragments appear designated as numbers within parentheses. Direction of each backbone appears marked by the 5′ and 3′ ends. Thus BP1 consists of two paired bases and the associated sugar-phosphate units (5) and (6), with similar notations used for BP2 through BP4. Phosphodiester linkages between nucleotide units exist between (5) to (7), (8) to (6), and so on.

Figure 2 shows a nucleotide fragment illustrating the definitions of the dihedral torsion angles applicable to the sugar-phosphate backbone and the glycosyl torsions. The sugar conformation, generally referred to as pucker, follows the convention set forth by Sundaralingham [54].

Figure 3 shows a B-DNA tetramer duplex. Figure 4 shows a model of the tetramer duplex DNA fragment that serves as the native Z-DNA structure for this study. A tetramer duplex is the

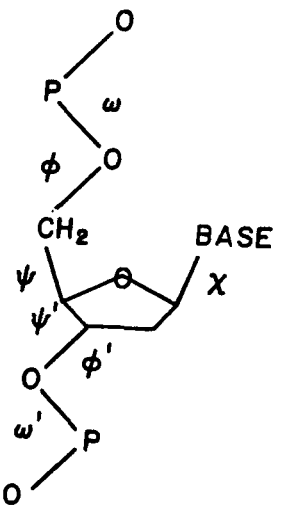

FIGURE 2 Schematic structure of a nucleotide fragment denoting the glycosyl and backbone torsion (dihedral) angles. Torsions are defined as follows: glycosyl torsion, χ_{pu}: C4-N9-C1′-C2′; χ_{py}: C2-N1-C1′-C2′; ω: O3′-P-O5′-C5′; ϕ: P-O5′-C5′-C4′; ψ: O5′-C5′-C4′-C3′; ψ': C5′-C4′-C3′-O3′ (sugar pucker); ϕ': C4′-C3′-O3′-P; ω': C3′-O3′-P-O5′.

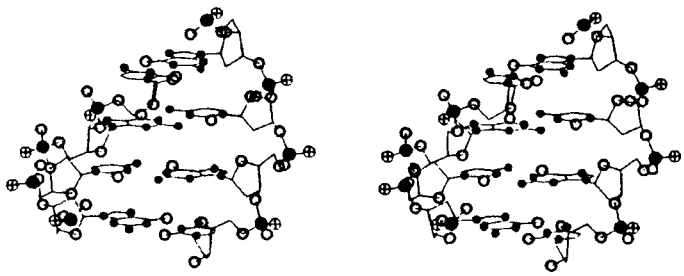

FIGURE 3 Stereo view of the B-DNA tetramer duplex consisting of four monomer repeat units. This is a fragment excised from a longer polymer unit. Viewpoint is into the major groove of the tetramer unit. The hydrogens are omitted for clarity.

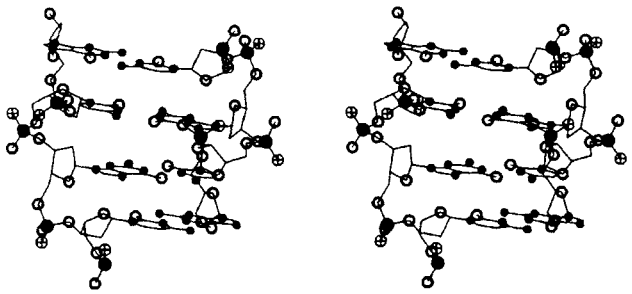

FIGURE 4 Stereo view of the Z-DNA tetramer duplex consisting of two dimer duplex repeat units. Viewpoint is into what was formerly the major groove of B-DNA. Hydrogens are omitted for clarity.

smallest fragment of Z-DNA containing both potential intercalation sites. This fragment is an excised piece of the dodecamer duplex Z-DNA comprising one complete turn of the helix. This convention originally applied to the B-DNA variants of earlier studies[29, 31, 33, 34, 37–42]. Parameters defining the native Z-DNA fragment appear in Table I.

RESULTS

Figure 5 illustrates a classical intercalation site of B-DNA, and the corresponding conformational data appears in Table I. The salient feature to note is the 5′-py-p-pu-3′ sequence, which appears in the X-ray crystallographic data of the known drug: DNA complexes referenced above.

TABLE I Conformational values of DNAs discussed

	χ_G	χ_C	ω	ϕ	ψ	ψ'	ϕ'	ω'
	Glycosyl and Backbone Torsion Angles (°)[1]							
B-DNA	130.9	130.9	−33.2	159.7	32.9	C2N	−162.0	−131.5
Z-DNA(CpG)[2]	−50.0	84.0	33.0	−124.2	−155.9	O4NI[3]	−100.6	120.0
Z-DNA (CpG)[4]	−50.0	84.0	−137.1	157.5	50.0	C2N	− 98.1	− 43.6
B-DNA (IC[5])	130.0	78.6	−134.1	−117.4	145.2	C3N	−177.6	−103.7
Z-DNA (GpC:IC)[6]	−53.0	50.0	−134.9	− 96.8	3.7	C1X	−168.3	− 67.9
Z-DNA (CpG)[7]	−53.0	50.0	91.5	−107.4	−162.9	C2N	178.8	174.8

[1] See Figure 2 and its caption for definitions.
[2] The Helical parameters of this dimer component are: α_z=−10.00°, ΔZ=3.80 Å, ΔX=−3.00 Å, α_y=−8.0°. See Ref. 41 for definitions.
[3] Z-DNA structures generally exhibit C1X or C3N conformations of this sugar ring. Other variants slightly different are supportive of Z-conformation also [40]
[4] The helical parameters of this dimer component are: α_z=−49.39°, ΔZ=3.80 Å, ΔX=−0.5 Å, α_y=−8.0°. See Ref. 41 for definitions.
[5] IC: Intercalation Site
[6] The helical parameters of this dimer component are: α_z=−10.3°, ΔZ=7.0 Å, ΔX=0.0 Å, α_y=0.0°. See Ref. 41 for definitions.
[7] The helical parameters of this dimer component are: α_z=−18.8°, ΔZ=3.8 Å, ΔX=−3.0 Å, α_y=0.0°. See Ref. 41 for definitions.

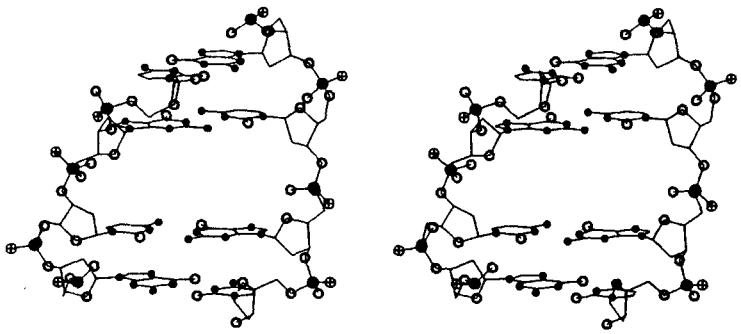

FIGURE 5 Stereo view of the B-DNA intercalation site viewed into the minor groove. Note the 5′-py-p-pu-3′ sequence between BP3 and BP2. Hydrogens are omitted for clarity.

In principle however, since the intercalation site also arises from factors residing in the backbone (dihedral angles) of the B-DNA, there is no structural reason the binding site cannot contain other sequences such as 5′-py-p-py-3′, 5′-pu-p-pu-3′, 5′-pu-p-py-3′. It is (only) specific drug: DNA interactions that dictate sequence preferences of the bases at the intercalation site in B-DNA as revealed by experimental data as cited above.

The presence of a repeating dimer duplex in Z-DNA provides two potential intercalation sites, site 2 that has a 5′-pu-p-py-3′ (*syn-anti*) sequence and site 1 that has a 5′-py-p-pu-3′ (*anti-syn*) sequence (Fig. 1). The base sequence at site 2 (5′-pu-p-py-3′) is different from that observed the B-DNA intercalation site (which has both bases in the *anti* configuration). Figure 6 illustrates a potential Z-DNA intercalation site. The corresponding conformational data for this site appear in Table I. The salient features of the Z-DNA intercalation site are two in number: (1) the Z-DNA intercalation site occurs at the *syn-anti* site that has the 5′-pu-p-py-3′ sequence not observed in classical B-DNA intercalation sites, (2) only one component of the Z-DNA dimer duplex is able to extend its backbone enough to accommodate an intercalant, i.e., it is conformationally polarized.

In the case of Z-DNA the alternating *anti-syn* conformation determines the intercalation site. Additionally, the sugar puckers play a role on Z-conformation as noted in ongoing theoretical studies of Z-DNA conformational domains [47]. Thus the sugar pucker sequence appears equally important with the *anti-syn* conformational properties of Z-DNA as judged by experimental [4, 9, 10] and theoretical studies [47].

DISCUSSION

Table II compares the torsion angle regions of the Z-DNA conformers and the B-DNA conformers. One of the arguments for the relative instability of Z-DNA compared to B-DNA is the closer approach of the phosphate groups of the sugar-phosphate backbone [55]. Two backbone torsion angles differ significantly between the B-and Z-intercalative conformers. The ψ angle shifts from the t^- region to the g^+ region and for ω', the shift is from t^- to g^-. These changes have the effect of slightly increasing the phosphorus-phosphorus atom distances at the intercalation site for the Z-conformer compared to the B-conformer intercalation structures. This effect is quantified in Table III and shown in Figure 7.

The intercalation conformation of Z-DNA identified in this study has the sequence 5′-pu-p-py-3′, the opposite as observed experimentally in the B-DNA conformer. Intercalation at the *anti-syn* (5′-py-p-pu-3′) site in Z-DNA is not

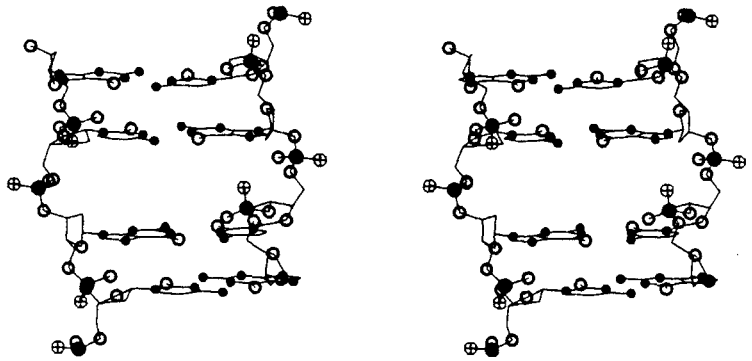

FIGURE 6 Stereo view of the Z-DNA intercalation site viewed into the formerly major groove. Note the 5′-pu-p-py-3′ sequence between BP3 and BP2, shifted from the B-DNA version of Figures 3 and 5. Hydrogens are omitted for clarity.

TABLE II Comparison of Z-DNA and B-DNA conformers

	χ_G	χ_C	ω	ϕ	ψ	ψ'	ϕ'	ω'
	Glycosyl and Backbone Torsion Angles Conformation Region[1]							
B-DNA	*anti*	*anti*	g^-	t^+	g^+	C2N	t^-	t^-
Z-DNA (CpG)	*syn*	*anti*	g^+	t^-	t^-	O4NI[2]	t^-	t^+
Z-DNA (GpC)	*syn*	*anti*	t^-	t^+	g^+	C2N	t^-	g^-
B-DNA (IC[3])	*anti*	*anti*	t^-	t^-	t^+	C3N	t^-	t^-
Z-DNA (GpC:IC)	*syn*	*anti*	t^-	t^-	g^+	C1X	t^-	g^-

[1]See Figure and its caption for definitions. $0° < g^+ < 90°$; $-90° < g^- < 0°$; $90° < t^+ < 180°$; $-180° < t^- < -90°$.
[2]Experimental Z-DNA structures exhibit C1X or C3N conformations of this sugar ring. Other variants slightly different are supportive of Z-conformation also [40].
[3]IC: Intercalation Site.

tenable for conformational reasons. Extension of the backbone along the helical axis to separate the base pairs is limited to a value much less than 6.8 Å, a value minimally required to accommodate a planar aromatic ring system between the adjacent base pairs at the intercalation site.

The data of Table II suggest backbone constraints coupled with glycosyl conformation play an important role in determining the intercalation site. In order to assume an intercalation conformation, extension of the sugar-phosphate backbone must occur. The first consideration is to recognize that in going from B- to Z-DNA, the base pairs are 180° aligned from what they are in B-DNA. If one looks at Figure 3 and draws a line between the 5′-P and the 3′-P, this line represents a virtual bond about which the sugar unit must be rotated to assume the Z-DNA orientation. This requires rotation around the glycosidic bond at site 2 (5′-G-p-C-3′), resulting in a *syn* conformation, while at site 1 (5′-C-p-G-3′) rotation of the entire base pair is required, which results in retention of the *anti* conformation but a drastic change in the conformation of the deoxyribose-phosphate backbone [2, 4]. Table II shows that the backbone torsion angles affected most by the conversion from B- to Z-DNA are ω, ψ, and ω'. These torsion angles also differ between the two sites of Z-DNA, resulting in a greater extension of the backbone torsions at site 1 in native Z-DNA. Thus for site 1, the 5′-C-p-G-3′ (anti-*syn*) site, any further extension leads to failure of closure of the backbone using GAGNAS, that is, the backbone will have disallowed bond angles and

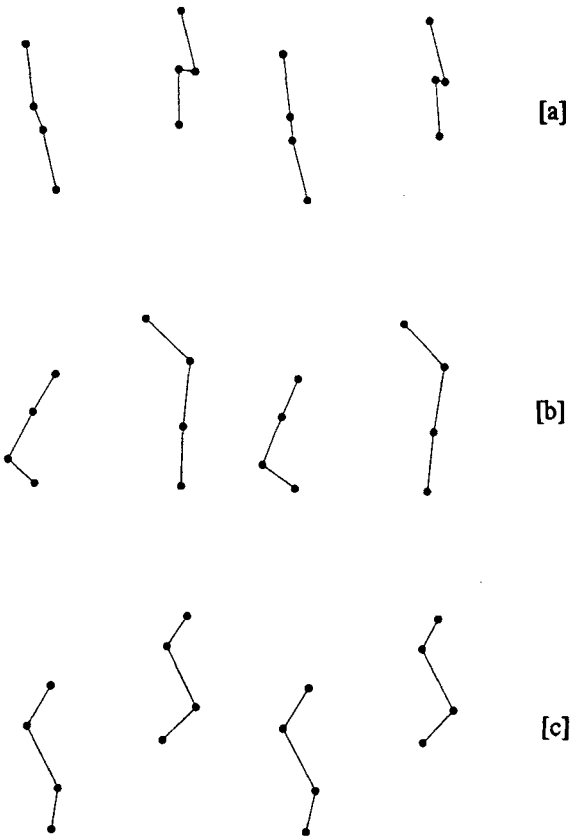

FIGURE 7 Stereo view of the comparison of the phosphorous atom plots of (a) B-DNA (IC), (b) Z-DNA, and (c) Z-DNA (IC). See Discussion.

bond lengths, [29] which indicates that further extension of the backbone is not possible in this Z-DNA site. The backbone of native Z-DNA at site 2 is not fully extended, which allows this site to accommodate intercalation. This change in the backbone torsion angles in the Z-conformer also changes the sense of extension of the backbone torsions required for assumption of an intercalation site in Z-DNA. In B-DNA, the torsions that change on assumption of the intercalation site are ω and ψ. In Z-DNA the torsions that change to accommodate intercalation for the G base nucleotide unit are ω, ψ, and ω'.

The X-ray crystallographic structure of Z-DNA is also consistent with a conformationally polarized binding site. A large shift occurs along the long axis of the base pair and a twist angle of $-9°$ at site 2. As a result there is no intrastrand stacking of the bases associated with this site. In contrast, at site 1 there is only a small amount of sheer accompanied by a helical twist of $-19°$, resulting in favorable intrastrand stacking interactions between C and G similar to those that stabilize B-DNA[1]. The differences in the backbone torsion angles of Z-DNA together with the absence of stabilizing intrastrand stacking interactions at site 2 make it more favorable energetically for the intercalation site to form at this site. Additionally, X-ray studies show that the minor groove is considerably larger at site 2 than at site 1 [1], which would facilitate the entry of intercalants at site 2.

Table III also lists the calculated energies of the four DNA conformers studied. The higher

TABLE III Intercalation site data for each DNA tetramer type

DNA Conformer	Energy[1] Kcal/mol	Intercal. Site Helical Angle[2]	Intercal. Site P-P Intrastrand[3] Distance	Intercal. Site P-P Interstrand[4] Distance
B-DNA	1189.3	+ 36.00°	6.69 Å	18.8 Å
Z-DNA (CpG)		− 10.00°	–	–
Z-DNA (GpC)	1595.7	− 49.39°	6.63 Å	16.5 Å
B-DNA (IC[5])	1348.4	+ 29.97°	7.29 Å	17.5 Å
Z-DNA (apC : IC)	1440.9	− 10.25°	7.40 Å	15.1 Å
Z-DNA (CpG)		− 18.75°	–	–

[1] ΔE[B(IC)-BDNA] = +159 Kcal/mol; ΔE [Z(IC)-ZDNA] = −155 Kcal/mol.
[2] For BP2 → BP3 helical rotation.
[3] P-P distance of sugar-phosphates (7) → (9). See Figure 2.
[4] P-P distance of sugar-phosphates (7) → (8). See Figure 2.
[5] IC: Intercalation Site.

energy for Z-DNA compared to B-DNA is consistent with the fact that B-DNA is the observed form of *in vitro* DNA. The data in Table III show that the calculated energies of the intercalation site structure of B-DNA is slightly higher than that of the corresponding native structure while the ΔE of the Z → Z-IC transition is −155 Kcal/mol. The small differences in the calculated energies suggest that these structures can exist transiently in absence of intercalants, perhaps through a wave propagating energy disturbance mechanism in the DNA as suggested by Sobell [56–58].

Of interest is the ΔE for the Z-DNA → Z-IC transition that results in a favorable ΔE of −155 Kcal/mole. For the transition from Z-DNA to the Z-IC conformer, the intrastrand distance increases by about 0.8 Å while the interstrand P-P distance decreases by about 1.4 Å. The overall effect is to decrease the P-P repulsion, which results in the lower energy of the Z-IC conformer. In addition, the base pairs separate in the Z-IC conformer. High resolution X-ray crystallographic studies of Z-DNA show that the first hydration shell of Z-DNA exhibits of a number of water-DNA hydrogen bonds [1]. Of particular interest are water molecules that bridge the O2 keto groups of the C residues of alternating strands, and water that links the N2 amino group of G with phosphate oxygens. On the outer surface of the Z-DNA there is a water bridge between the O6 keto groups of G in site 1. There are also water molecules linking the phosphate groups, however this water is not as structured as the water around the bases. The 5′ and 3′ phosphate groups of the G residues are usually linked by two bridging water molecules. The increase in distance between the phosphate groups along with the separation of the bases that occurs in formation of the Z-IC conformer disrupts the water structure in the first hydration shell, providing an unfavorable contribution to the overall energy change resulting from formation of the Z-IC complex. Consequently, it is likely that the overall energy change for formation of the Z-IC conformer is actually positive.

Another interesting point concerning the intercalation site properties of the B- vs. Z-forms of DNA is the observed effect on the helical winding angles. For B-DNA the helical winding angle for repeat fragments (monomers) is 36°. For the B-IC conformer, the intercalation site exhibits a helical winding angle of 29.97°, or an unwinding of 6°.

In Z-DNA the helical winding angle for repeat fragments (dimers) is about −60°. For the Z-IC conformer, since two nucleotides comprise the repeat unit of native Z-DNA, we examine the helical winding angle of each monomer component of the dimer repeat unit. At the intercalation site itself, BP2 → BP3, the helical winding angle is −10°, little different from the corresponding site of the native Z-DNA structure of Figure 4 and Table I. What is interesting is that

the fragment below the Z-intercalation site, BP1 → BP2, exhibits a helical winding angle of −18.75° compared to a value of −49.4° in native Z-DNA. Formation of the Z-IC conformer winds the helix by about +31° and the winding is not localized at the actual intercalation site, but at the residue below it. Thus, B-IC structures show an unwinding of B-DNA at the intercalation site, but Z-IC structures exhibit a winding of the Z-DNA at the nucleotide residue trailing the intercalation site.

A final point concerns the neighbor exclusion principle in which once an intercalation site arises, adjacent sites are disallowed or excluded from assuming an intercalation conformation. This concept arose in examining the intercalation complexes of B-DNA noted above and has been discussed in some detail [30, 59–62]. The essence of the neighbor exclusion principle is that an intercalation site influences neighboring site conformations. Under this principle the intercalation site actually spans not 6.8 Å of the site proper, but 10.2 Å (6.8 Å+3.4 Å) which includes a neighboring duplex unit. Winding of the Z-DNA at the site adjacent to the intercalation site in the Z-IC structure is therefore consistent with the neighbor exclusion principle. Experimental X-ray fiber diffraction of a platinum terpyridine saturated calf thymus DNA exhibited the 10.2 Å meridonal reflections consistent with the 6.8 Å+3.4 Å intercalation site duplex [59]. Arnott *et al.* reinterpreted the platinum terpyridine complex data [61]. They argue that the 10.2 Å length of the intercalation site duplex is a result of significant differences in the glycosyl torsions and the sugar conformations (puckers) of the nucleotide units bounding the site. The platinum terpyridine complex exhibits a 5′-*anti*: C2N-p-*syn*: C3N-3′ trait using the convention of Figure 1. These parameters occur in what is a B-DNA variant, a right-handed helical structure. The intercalation site in the Z-DNA model proposed here adopts the opposite conformational trait, i.e., 5′-syn: C1X-p-anti: C2N-3′. The neighbor exclusion principle is well documented for B-DNA intercalation complexes, and the results presented in this paper indicate that it holds for the Z-DNA counterpart. Consequently, intercalation represents a case of allosterism in nucleic acids, i.e., a significant conformational change at one locus results in specific conformational changes that inhibit intercalant binding to an adjacent locus [63]. This is supported by the finding that intercalation causes the transition of Z- to B-DNA in a region containing from 5 to 25 base pairs around the intercalation site [64–66]. Generally, Z-DNA intercalation conformation results in the opposite traits observed in B-DNA intercalation conformations.

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[49] CompuAdd C466D, 486DX2, 540 Mbyte Hard Drive, 12 Mbyte RAM, 2 Mbyte Video RAM.
[50] Fortran Power Station, 32 bit, Version 1.0 a, Microsoft Corp.
[51] PC version of Mainframe software, beta test, Computer Associates.
[52] The helical parameters of the DNA are defined in ref. 29. Briefly, α_z, is the helical angle, α_y is the tilt of adjacent base pairs as measured about the Y-axis, ΔZ is the step height, ΔX and ΔY are the translations of adjacent base pairs measured relative to the X- and Y-axes, respectively. α_x is the tilt of the base pairs about the X-axis (also called the kink angle in refs. 38, 39, and 42).
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