Characterization of the Base Stacking Interactions in DNA by Means of Lennard-Jones Empirical Potentials

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Abstract. Three empirical potentials of the Lennard—Jones type taken from literature were used to calculate van der Waals contributions to the base-pair couples stacking energies in B-DNA and A-DNA type double helical conformations. The information obtained can be summarized as follows: (1) Purine-pyrimidine and purine-purine (pyrimidine-pyrimidine in the complementary strand) sequences preferred right-handed helical arrangement, whereas pyrimidine-purine sequences favoured left-handed (C—G) or unwound (T—A) stacking geometry; in the latter case this only held for B- but not A-DNA (the C—G sequence was not studied in A-DNA owing to difficulties (see below) with the G amino group in B-DNA); (2) Positive propeller twist of base-pairs was stable in both B- and A-DNA; the thymine methyl group promoted the propeller and this effect was strongest in the A—T step; (3) Tilt of base pairs occurred around zero in B-DNA and between 15—20 °C in A-DNA, in agreement with the experimental observations; (4) Vertical separation of base pairs was optimal within 0.33—0.34 nm for B-DNA and around 0.29 nm for A-DNA using the 9—6 potential. The 12—6 potential gave similar results with B-DNA as the 9—6 potential if, however, base pairs were separated by 0.35—0.36 nm; (5) The calculated effect of the guanine amino group was substantially stronger than expected on the basis of data derived from X-ray diffraction studies of oligonucleotide single crystals; (6) In comparison with the 9—6 potential, the 12-6 potential provided more strict energy minima. In summary, the empirical potentials reproduce, at least semiquantitatively, many but not all DNA properties; this should be taken into account whenever the potentials are used for prediction purposes.

Key words: DNA conformation — Base sequence — Base stacking — Empirical potentials

Introduction

Conformation and other physical properties of DNA determine which genomic nucleotide sequences are recognized by specific proteins that control and regulate gene expression, replication and recombination. The properties are often dramatically dependent on even a few of the DNA constituent atoms or chemical groups and it is thus necessary to study DNA at atomic resolution. However, experimental methods providing such a detailed information are very expensive and time-consuming to use. Evidently, principles should be extracted from the available experimental data which would allow predicting biologically relevant properties of DNA from its base sequences.

Even short DNA double helices are geometrically very complex if all their atoms are considered. The recent finding that the DNA sugar-phosphate backbone is very flexible and conformationally passive (Srinivasan and Olson 1987) while base stacking forces determine the biologically interesting sequence-dependent variations in the DNA double helix architecture (Dickerson 1983; Calladine 1982; Shakked and Rabinovich 1986) has substantially simplified the problem. Various empirical potential energy functions have been developed for the description of base stacking interactions in DNA (Gupta and Sasisekharan 1978; Lifson et al. 1979; Hagler et al. 1979; Haran et al. 1984, 1987; Tung and Harvey 1984, 1986); it should be decided which of the calculated properties are dependent on the potential choice and which are not. This is one point addressed in the present paper. Another aim is to evaluate the base-sequence and local geometry dependences of the stacking energy in the framework of the global B- and A-DNA conformations. These results will be used to analyze longer DNA fragments at a later date. We also dealt with Z-DNA and found that, unlike B- and A-DNAs, its stabilization energy did not originate from the base stacking interactions. Owing to this Z-DNA will not be discussed in this paper.

Two more comments are worthwhile before proceeding to the next section. Firstly, stacking energy involves van der Waals and electrostatic terms. The latter will be ignored in the present calculations as it only contributes less than 15 % to the total stacking energy and, even more important, it is insensitive to local geometry modifications (Haran et al. 1984). Secondly, there is a number of parameters defining base position in the DNA double helix. Not all of them, however, present equal contributions to the energy when changed within the variability limits indicated by the experimental data. Owing to this, only the energy dependences on the conformational parameters of the double helix will be analyzed which are the primary source of the base sequence-dependent conformational variations. The key parameters include position of the double helix axis with respect to the base pairs, their tilt, base pair separation along the helical axis, propeller twist and helical twist. On the other hand, conformational

Table 1. Atomic coordinates of base pairs[a].

Guanine	X	Y	Cytosine	X	Y
H-1	0.64	−0.73	N-1	4.57	−1.24
N-1	−0.45	−0.92	C-2	3.26	−1.46
C-2	−0.92	−2.16	N-3	2.42	−0.44
N-3	−2.23	−2.38	C-4	2.88	0.81
C-4	−3.07	−1.36	C-5	4.19	1.21
C-5	−2.61	−0.11	C-6	5.04	0.00
C-6	−1.30	−0.11	O-2	2.82	−2.62
N-7	−3.66	0.72	N(amino)	2.03	1.84
C-8	−4.75	0.00	H′(amino)	0.95	1.66
N-9	−4.41	−1.30	H″(amino)	2.42	2.87
N(amino)	−0.07	−3.18	H-5	4.57	2.06
H′(amino)	1.02	−3.00	H-6	6.12	0.18
H″(amino)	−0.45	−4.21			
H-8	−5.74	0.48			
O-6	−0.91	1.15			
Adenine			Thymine (Uracil)		
N-1	−0.46	−0.92	N-1	4.57	1.24
C-2	−0.92	−2.17	C-2	3.26	1.46
N-3	−2.24	−2.38	N-3	2.42	−0.44
C-4	−3.08	−1.36	C-4	2.88	0.81
C-5	−2.62	−0.11	C-5	4.19	1.03
C-6	−1.31	0.11	C-6	5.04	0.00
N-7	−3.66	0.72	O-2	2.82	2.62
C-8	−4.77	0.00	H-3	1.32	−0.62
N-9	−4.42	−1.30	O-4	2.09	1.77
H-2	−0.23	−3.01	Methyl[b]	4.71	2.43
H-8	−5.76	0.48	(H-5)[c]	4.57	2.04
N(amino)	−0.84	1.36	H-6	6.12	0.18
H′(amino)	−1.54	2.21			
H″(amino)	0.25	1.54			

[a] Standard geometries are presented (Tung and Harvey 1986) in which base pairs are ideally planar objects; the unit length is 0.1 nm.

[b] The thymine methyl group is represented by a single extended atom.

[c] This row concerns uracil.

parameters giving relatively small values in experimentally determined structures or those variations which little change energy, as determined by our preliminary calculations, will be set zero throughout this article. These parameters include base pair roll, buckle and slide.

Table 2. Force field constants of the various Lennard-Johnes empirical potentials used in the present study[a)]

9—6 LH			12—6 LH			12—6 TH		
Atom	$B \times 10^4$	$A \times 10^3$	Atom	$B \times 10^5$	$A \times 10^3$	Atom	$B \times 10^5$	$A \times 10^3$
C	1.63	5.15	C	3.40	2.23	C	1.68	7.50
H_C	0.0186	0.063	H_C	0.003	0.14	Methyl	3.38	7.14
C_O	0.52	1.49	C_0	1.27	5.61	H	0.0046	0.18
N	3.64	8.46	N	0.95	5.15	M[b)]	0.89	5.72
O	1.92	5.90	O	0.0115	2.1	N[c)]	1.68	7.50
						O	0.14	1.54

[a)] Hagler—Lifson (LH) potential distinguishes between C attached to H and C attached to O whereas no discrimination is made between ring and amino N. The Tung—Harvey (TH) potential takes all C's identical but a difference is made between ring and amino N's. Values A_{ij} and B_{ij} introduced in equation (1) are square roots of the products of the corresponding constants A and B characterizing the participating atoms i and j. The constants B and A are expressed in kJ nm^9 mol^{-1}.l and kJ nm^6 mol^{-1}.l, respectively, for 9—6 LH. For 12—6 LH and 12—6 TH, the corresponding units are kJ nm^{12} mol^{-1}.l and kJ nm^6 mol^{-1}.l.

[b)] M is nitrogen in the amino group.

[c)] N is ring nitrogen.

Materials and Methods

The geometry of base pairs was deduced from the work of Tung and Harvey (1986); the atomic coordinates are shown in Table 1.

The van der Waals part of the base stacking energy has the form of a Lennard-Jones type function and there is a widely accepted understanding that its atractive part is proportional to the inverse sixth power of the interacting atoms separation. On the other hand, it still remains unclear whether the repulsive part is better described by a term proportional to the inverse ninth or twelfth power of that distance. The latter variant is physically better interpretable but the former gives a better agreement with the experimental data (Hagler et al. 1979). We use three potentials in this work. The first two were derived from crystal data on simple organic compounds by Lifson and coworkers (1979) (further referred to as LH). One of the potentials has the repulsive term dependent on the inverse ninth power of the interatomic distance and was used by Haran et al. (1984) to analyze van der Waals parts of the base stacking energies in the known crystal conformations of B- and A-DNA fragments. The other potential has a 12—6 character (Lifson et al. 1979). The third is also of the 12—6 type and was used by Tung and Harvey (1986, further referred to as 6—12 TH) in their theoretical studies of the sequence dependence of local geometry of B-DNA double helix. Force field constants of all the three potentials are summarized in Table 2. Van der Waals energy E of a base pair couple is calculated using the expression

$$E = \sum_{i,j} (A_{ij} r_{ij}^{-6} + B_{ij} r_{ij}^{-9, \text{ or } -12}) \qquad (1)$$

where the constants A_{ij} and B_{ij} are geometrical averages of the corresponding force field constants (Table 2), characterizing the involved pairs of atoms i and j, r_{ij} is their distance. The thymine methyl

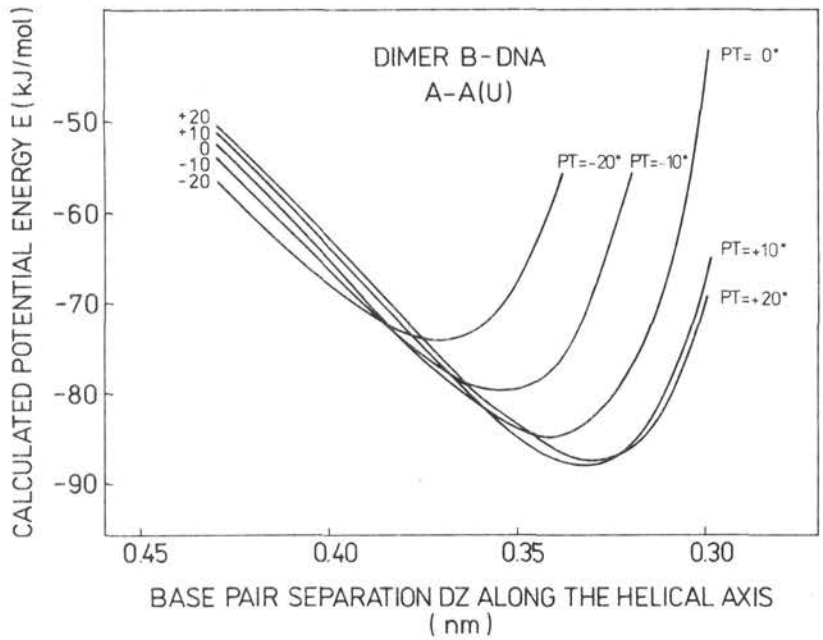

Fig. 1. Dependence on DZ of the calculated potential energy E (using the 9—6 potential of Lifson and Hagler) for an A—A dimer (U—U in the complementary strand) in B-DNA geometry (BR = TI = 0°, HT = 36°) for various values of PT.

group is represented by a single extended atom. Its van der Waals parameters are not presented in 6—9 LH so that we use the values which reproduce the minimum of 6—12 TH.

All reported calculations were run on an ICL 2950/10 computer of the Regional Computing Centre of the Czechoslovak Academy of Sciences, Brno. The software was written in a slightly modified version of Fortran 77.

Results and Discussion

B-DNA Global Geometry

Within the framework of typical geometry of B-DNA, van der Waals stacking energies of all possible doublets containing either GC (IC) or AT (AU) base pairs were examined and their energy dependences on TI, DZ, PT and HT were determined. From the calculations, several general conclusions could be drawn. First, in B-DNA global geometry which is typical by base pairs located in the double helix centre, TI is close to zero in the most stable conformations of all sequences, and DZ generally lies between 0.33 and 0.34 nm, if the 9—6 potential

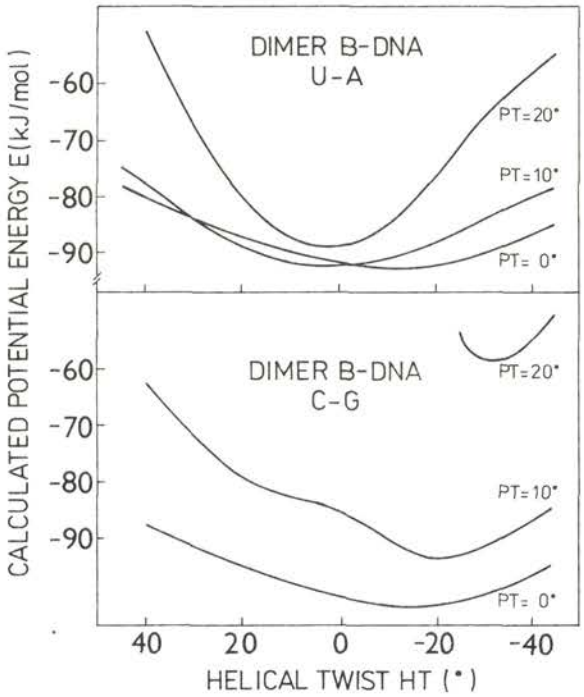

Fig. 3. Dependence of E (9—6 LH) on HT (PT is a parameter) for the indicated base pair dimers in B-DNA. TI = BR = 0°, DZ = 0.34 nm.

U. In alternating sequences the two U's on different strands in successive base pairs did not interfere at all, while a clash occurred between their complementary A's at PT > 10°. This clash was stronger in the U—A step as compared to A—U step so that, naturally, the former step is expected to be less propeller twisted, which has actually been observed (Shakked and Rabinovich 1986). The same tendencies were also observed with sequences containing GC base pairs, with the following modifications. Firstly, in the G—G sequence the difference between the repulsion of 5'end purine and 5'end pyrimidine and of the reverse couple was diminished. Secondly, in the G—C step the interpurine clash at positive PT was weaker than in the A—T sequence while in the C—G it was much stronger than in T—A.

A-DNA Global Geometry

With A-DNA our calculations gave energy curves containing more strict minima than with B-DNA; however owing to the unexplained problems with the

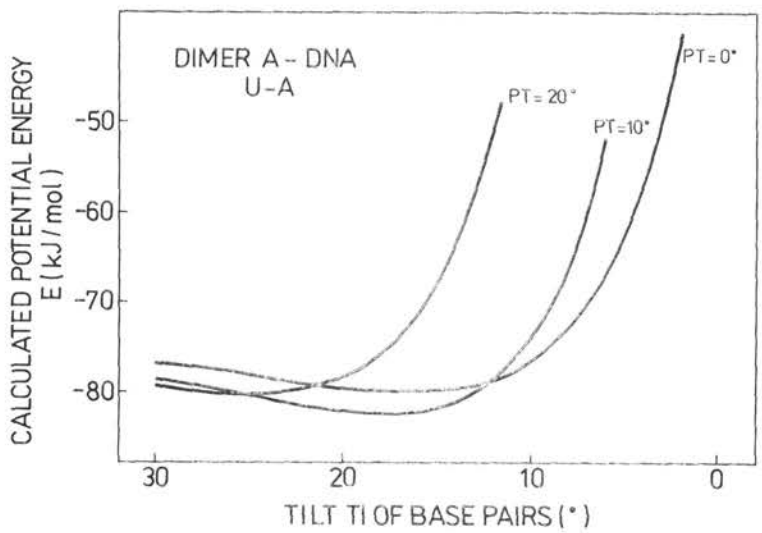

Fig. 4. Dependence of E (9—6 LH) on TI for the U—A dimer in A-DNA at the indicated values of PT. HT = 30°, DZ = 0.29 nm, BR = 0°.

amino group of G (see above) we mainly considered sequences containing AT or AU base pairs. On the other hand, we assume that our results obtained for AT and AU sequences in A-DNA correctly reflect the actual situation as A-DNA is known to be less conformationally variable than B-DNA (Dickerson 1983). Then it is natural that the stacking energy curves of base pairs in A-DNA show better defined minima. Our calculations mainly reproduce the observed tilt of base pairs in A-DNA for various values of PT and the step U—A (Fig. 4).

Values of PT lying within 0—10° require TI higher than 10° while if PT = 20°, then TI is also at least 20°. Relevant information concerning stabilities of A—A (U—U), A—U and U—A base pair couples in A-DNA type arrangements characterized by various values of HT, DZ and PT are summarized in Table 3. Besides TI, our calculations also reproduce the experimentally observed positive PT in A-DNA single crystals. Figure 5 shows the energy dependence obtained for A—T sequence using the 9—6 potential of Lifson and Hagler in A-DNA global geometry in which HT is variable and PT a parameter. The favourableness of PT values between 10—20° is obvious. The optimum of HT is, as with B-DNA, at rather lower angles than observed in crystals so that stacking forces evaluated using the 9—6 potential of Lifson and Hagler tend to unwind the A-DNA double helix. Optimum values of HT for various fixed values of PT and various base pair dimers are summarized in Table 4. It follows

Table 3. Optimum values of base pair tilt (oTI) and the corresponding potential energy E (in kJ mol^{-1}.l) obtained using the 9—6 potential of Hagler and Lifson for A—A (U—U in the complementary strand), A—U and U—A base pair couples in A-DNA global geometry in dependence on helical twist (HT) and base pair separation (DZ).

Dimer	HT	DZ	PT = 0°		PT = 10°		PT = 20°	
			oTI	E	oTI	E	oTI	E
A—A	36	0.3	10	−79.1	10	−79.3	14	−75.8
A—A	30	0.3	12	−83.3	14	−83.3	15	−82.5
A—A	36	0.29	12	−79.3	12	−80.2	14	−77.0
A—A	30	0.29	16	−82.5	20	−81.6	16	−84.2
A—U	36	0.3	13	−80.4	8	−80.8	8	−80.2
A—U	30	0.3	15	−85.6	12	−85.8	9	−85.4
A—U	36	0.29	15	−80.6	11	−81.0	10	−80.6
A—U	30	0.29	20	−86.0	16	−86.2	13	−85.6
U—A	36	0.3	8	−77.0	12	−77.7	18	−73.7
U—A	30	0.3	12	−80.2	14	−81.9	23	−78.9
U—A	36	0.29	12	−77.0	14	−82.7	20	−75.2
U—A	30	0.29	16	−80.2	18	−82.1	26	−80.6

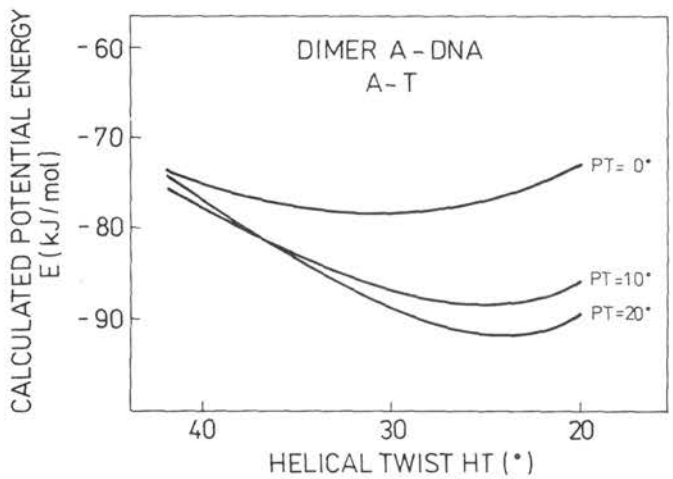

Fig. 5. Dependence of E (9—6 LH) on HT for the indicated values of PT of an A—T dimer in A-DNA conformation. TI = 17°, BR = 0°, DZ = 0.29 nm.

from this Table that stacking in the G—C step is stronger than in C—G, A—T and T—A steps in A-DNA geometry and that its arrangement and stability are only marginally dependent on PT within 0—20°. It is further interesting that C—G and T—A steps are destabilized by large positive PT while A—T step

Table 4. Stacking energy values (E in kJ mol^{-1}.l) and helical twist (HT) for optimum A-DNA arrangements of various base-pair dimers (DZ = 0.29 nm, TI = 7°)[a]

Dimer	PT = 0°		PT = 10°		PT = 20°	
	HT	E	HT	E	HT	E
C—G	25	−90.2	28	−89.0	39	−76.6
G—C	26	−95.9	24	−97.8	23	−97.3
T—A	24	−85.0	24	−86.7	32	−76.0
A—T	31	−78.3	25	−88.6	24	−92.1
A—A[b]	37	−107.2	34	−112.2	32	−112.6

[a] Except for the A—A base pair dimer, where the 12—6 potential of Tung and Harvey was employed, all other energies in this Table were calculated using the 9—6 potential of Lifson and Hagler.

[b] U—U in the complementary strand.

Table 5. The effect of TI, DZ and PT on the stability of A-DNA (HT = 30°). Energy E is in kJ mol^{-1}.l.

Dimer	Potential	DZ = 0.29 nm			0.27 nm			0.256 nm		
		E	TI	PT	E	TI	PT	E	TI	PT
A—A	9—6 LH	−84.4	16	20	−82.3	22	20	−75.8	24	20
A—U	9—6 LH	−86.2	16	10	−85.0	22	10	−80,0	25	10
U—A	9—6 LH	−82.5	18	10	−83.1	24	10	−81.0	28	10
A—A	12—6 TH	−114.3	20	20						
A—A	12—6 LH	−60.3	20	20				−32.2	28	20

shows an opposite tendency. A—A (U—U) step is stable irrespective of whether PT is 0, 10 or 20°; this and the previous data however cannot be compared as they were obtained for different potentials.

As far as DZ is concerned, its optimum values fall in the range 0.29—0.27 nm (Table 5).

Use of Different Empirical Potentials

To make an image on the validity of the results reported above we performed some calculations using all the potentials described in Materials and Methods on various sequences of AU base pairs, mainly in the B-DNA global geometry. The first and important conclusion following from these calculations is that in several respects the calculated sequence-dependent effects are less than differences among the results obtained using various potentials. On the other hand, a number of results remain invariant regardless of the potential.

Table 6. Optimum values of helical twist for various base pair dimers obtained using different potentials in B-DNA global geometry (TI = BR = 0°). In each case, PT adopts one of the values ± 20°, ± 10° or 0° for which the base pair arrangement is the most stable.

Potential	DZ (nm)	A—A[a]	A—U	U—A	G—G	G—C	C—G	I—I	I—C	C—I
6—9 LH	0.34	17°	15°	5°	17°	17°	−15°	17°	17°	−15°
6—12 LH	0.34	35°	30°	27°	37°	40°	40°			
6—12 LH	0.34	35°	35°	32°	27°					
6—12 LH	0.36	22°	17°	12°						

[a] U—U in the complementary strand

Table 7. Optimum values of propeller twist for various base pair dimers obtained using various potentials in B-DNA global geometry (DZ = 0.34 nm, HT = 40°, TI = BR = 0°).

Potential	A—A[a]	A—U	U—A	G—G	G—C	C—G
6—9 LH	12°	0°	4°	4°	4°	0°
6—12 LH	18°	12°	0°			
6—12 LH	18°	12°	0°			

[a] U—U in the complementary strand.

Generally, the energy curves obtained using 12—6 potentials have better defined minima at DZ = 0.34 nm than those obtained by means of the 9—6 potential. The 12—6 potentials give optimum HT (Table 6) and PT (Table 7) very close to experimental data. There are steep barriers to changes at these optimum values. However, the effect of the G amino group is even enhanced by replacing the 9th by 12th power in the repulsive part of the Lennard—Jones potential. Another natural consequence of this replacement is a shift of the optimum DZ values from 0.33—0.34 nm to 0.345—0.36 nm. TI remains approximately zero in B-DNA. Results obtained using the 12—6 potential of Tung and Harvey are very similar to those following from the use of the 12—6 potential of Lifson and Hagler if the latter energy values are multiplied by a factor of about 2.5.

In an attempt to improve the correspondence of the results obtained using the 9—6 and 12—6 potentials we made an interesting observation: the 9—6 and 12—6 potentials of Lifson and Hagler gave very similar energy curves if DZ was 0.34 nm in the former case but 0.36 nm in the latter. Under this condition, the calculated sequence-dependent effects were invariant with respect to the potential (Fig. 6). Tung and Harvey (1986) have used a 12—6 potential in their study; in view of our results it is therefore hardly justified to set DZ to 0.34 nm though

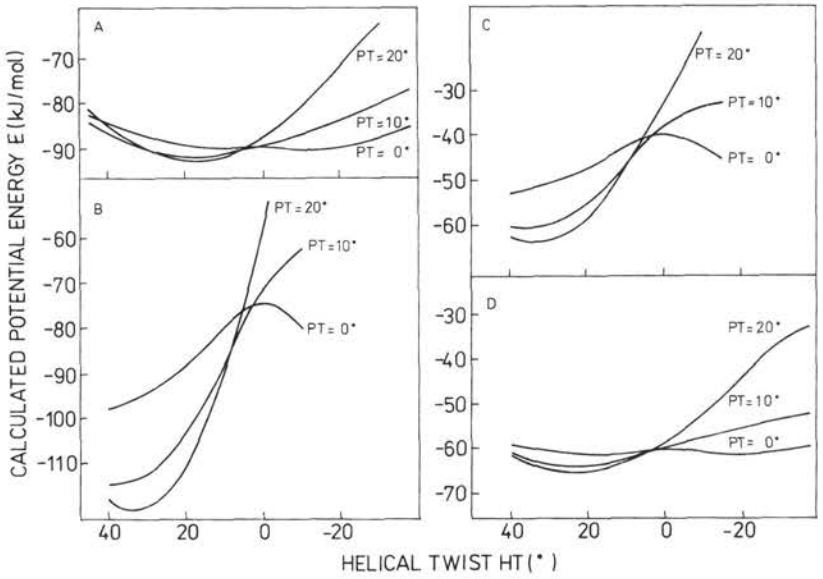

Fig. 6. A comparison of the dependences of potential energy E on HT for B-DNA geometry (TI = BR = 0°, DZ = 0.324 or 0.36 nm, PT = 0°, 10° or 20°) with an A—A (U—U in the complementary strand) dimer calculated using different potentials and values of DZ: *A*) 9—6 Lifson and Hagler, DZ = 0.34 nm; *B*) 12—6 Tung and Harvey, DZ = 0.34 nm; *C*) 12—6 Lifson and Hagler, DZ = 0.34 nm, and *D*) 12—6 Lifson and Hagler, DZ = 0.36 nm.

this value is in agreement with most experimentally obtained values of DZ in B-DNA.

Prediction Strength of the Empirical Potentials

Generally, the employment of the empirical potential for the analysis of DNA sequence-dependent properties is more controversial than it might seem from some recently published papers (Haran et al. 1984; Tung and Harvey 1984, 1986). First of all, not all calculated properties are invariant with respect to the potential choice. The potential-dependent differences in some results are larger than the calculated sequence-dependent properties. As far as DZ is concerned, the 9—6 potential better reproduces the actual state than does the 12—6 potential. The same is believed to be true for HT as exact reproducibility with 12—6 potentials of experimental values by merely considering base stacking interaction is hardly realistic. Interphosphate interactions in the polynucleotide backbone modulated by solvent conditions are certainly also an important

factor which contributes to double-helical folding of DNA as otherwise salt or alcohol-induced isomerizations of DNA double helices could not be observed (Vorlíčková and Kypr 1985a,b; Jovin et al. 1987). In addition, flatness of the energy curves obtained using the 9—6 potential appears to fit better into the picture of dynamic DNA derived from NMR studies (Kearns 1984) than the curves obtained using the 12—6 potentials characterized by strict minima.

We find that a substantial problem is introduced in the calculations concerning DNA base pairs by the G amino group. Its empirical potential seems inadequately strong, which holds irrespective of the potential used. On the other hand, the potentials adequately describe forces operating in crystals of simple organic compounds of which they derive. Work is in progress to explain this apparent contradiction.

Above, problems of shortcomings were summarized of the use of Lennard-Jones type empirical potentials to describe vertical interactions of bases and to take the results as a basis to predict the whole DNA conformation. Now we shall focus on positive aspects of this approach. The calculations are in a reasonable accordance with experimental data for B- and A-DNA as far as TI and PT are concerned. DZ is also reasonably reproduced in both B- and A-DNA, and an interesting finding is that the optimum value of this parameter depends on the potential choice. Calculated values of HT do not exactly correspond to the values found for single crystals of DNA fragments but it is not excluded that they suggest DNA properties that are authentic though not yet properly experimentally documented. We mainly think of the left-handed arrangement of DNA at C—G steps with the base pair topology of B-DNA, i.e. not Z-DNA, and an unwound arrangement of DNA at T—A steps. The main conclusion of the present study is that empirical potentials are not yet a reliable predictor of base-sequence variations in some B- and A-DNA conformational parameters (DZ, HT). On the other hand, they correctly predict some other DNA properties (TI or PT) and it is only a matter of accumulation of a larger body of experimental data to provide a reference for potentials which can then be precised to become a valuable tool for DNA conformation studies.

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List of Symbols

A, C, G, T, I and U — bases of nucleic acids
E — base stacking energy in kJ mol^{-1}.l
AU — hydrogen bonded adenine with uracil
A—U — adenine followed by uracil in the same strand

DX, DY, DZ, HT, PT, TI — conformational parameters describing the position of bases in the DNA double helix. DX and DY specify base pair position with respect to the helical axis, DZ is vertical separation of neighbouring base pairs. HT, PT and TI stand for helical twist, propeller twist and tilt of base pairs, respectively.

6—12 TH, 6—12 LH, 6—9 LH — Lennard—Jones empirical potentials describing the van der Waals part of the base stacking energy in DNA. The numbers reflect the inverse interatomic distance powers in the attractive and repulsive terms of the potentials, respectively. The letters stand for Tung and Harvey or Lifson and Hagler who developed or employed the particular potentials.

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