

Hydrogen bonding between water molecules

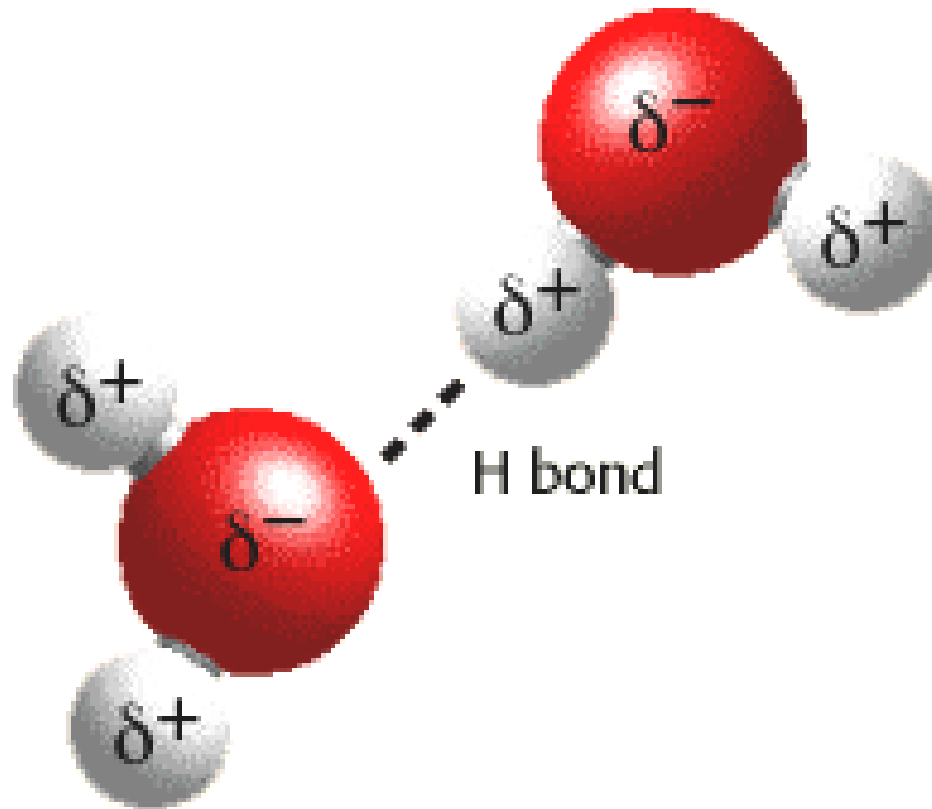
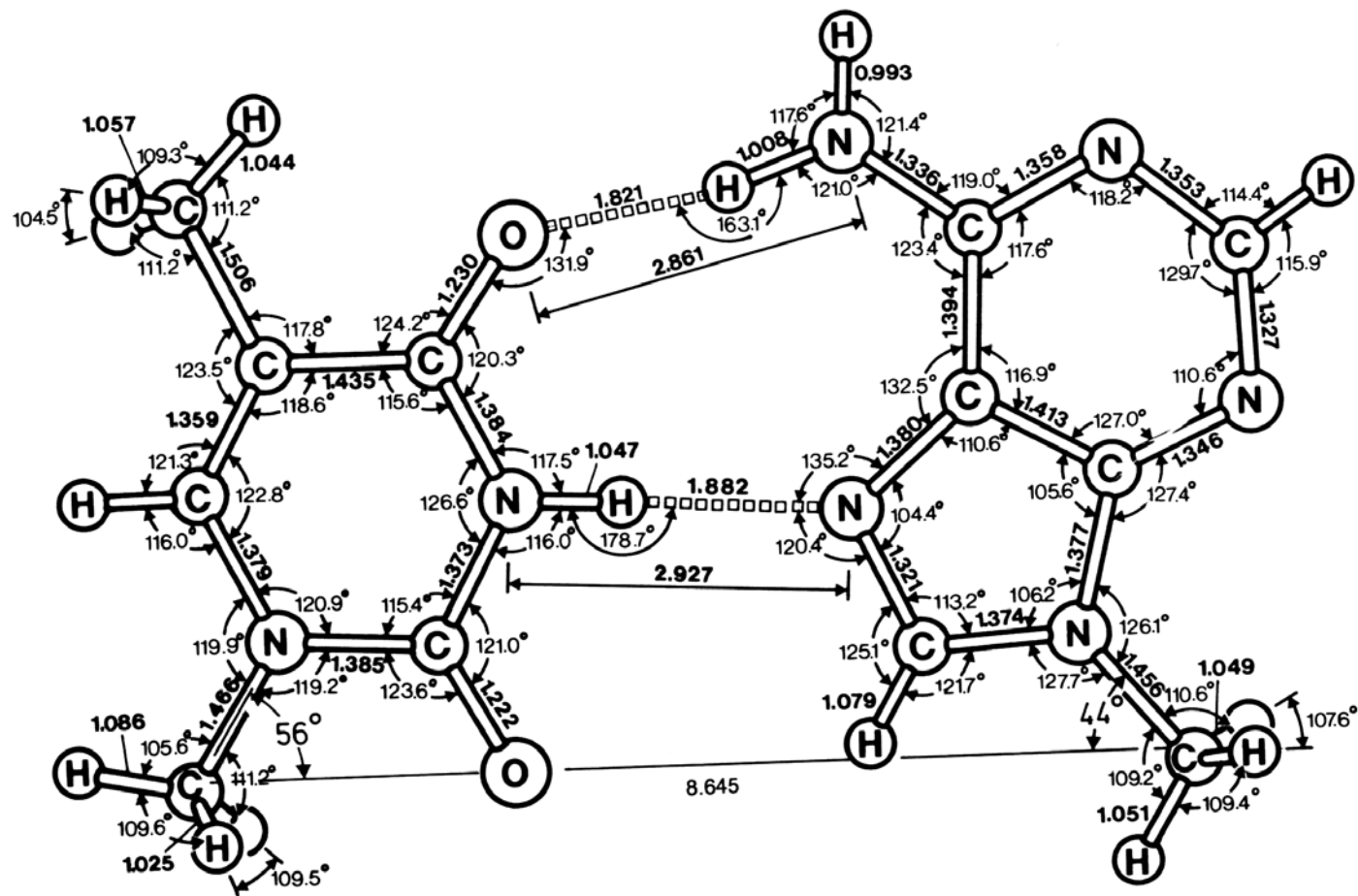
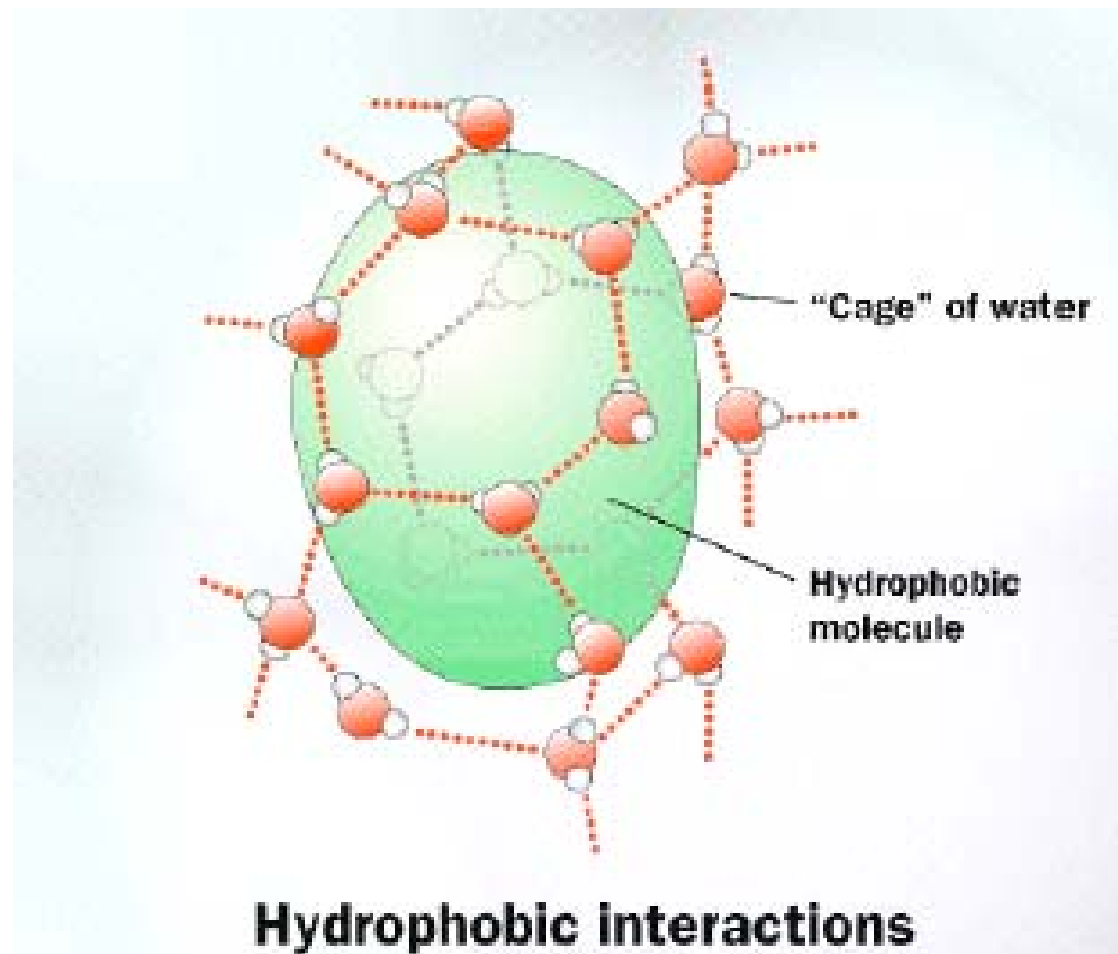


Table 6-1. Comparison of Some Energy Values in Covalent and Hydrogen Bonds

Bond type	Bond length Å	Bond energy kcal/mole	Energy required for lengthening by 0.1 Å kcal/mole
Covalent			
C—C	1.54 ± 0.02	83.1	3.25
C—H (in ethane)	1.09 ± 0.02^a	98.8 ^b	3.60 ^c
Hydrogen bond			
O—H . . . O	2.75 ± 0.2^d (O . . . O distance)	3 to 6 ^e	0.1 ^f





Time

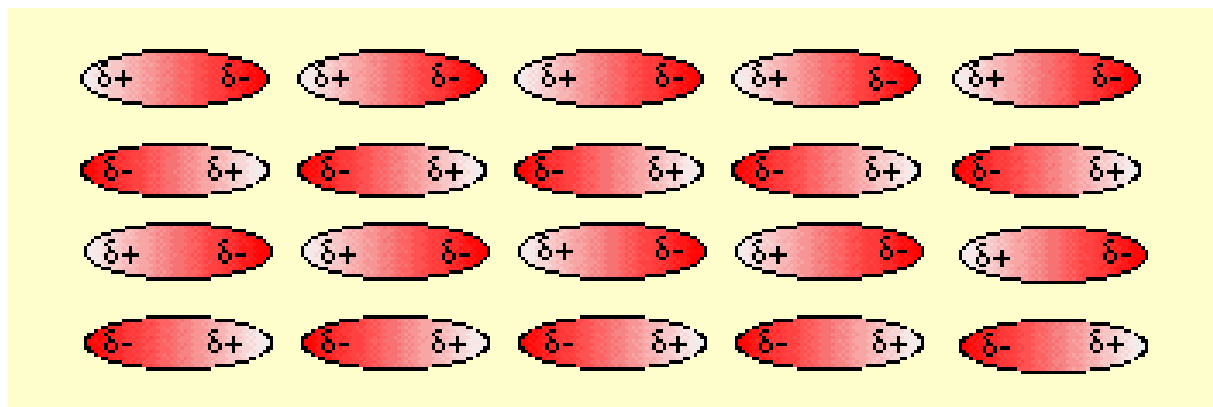
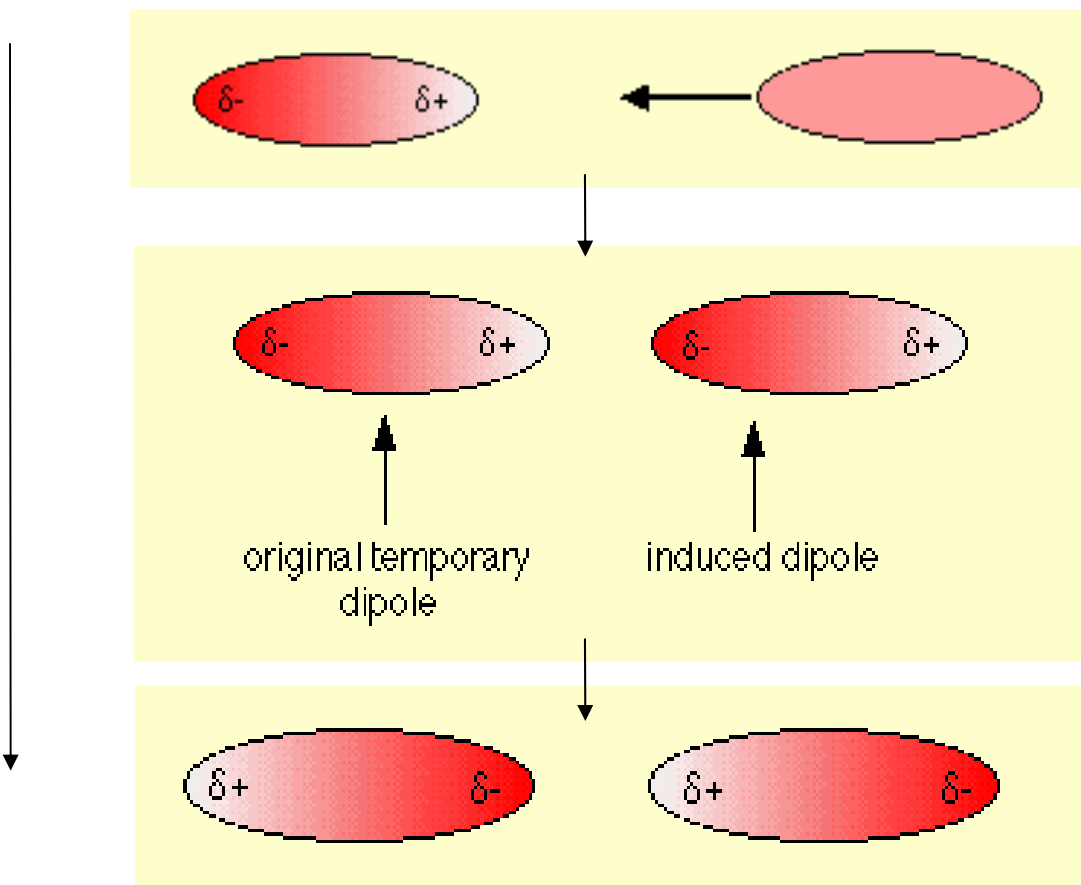
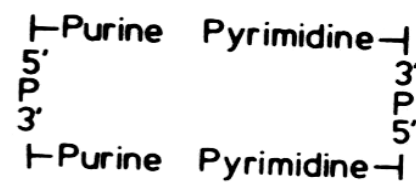
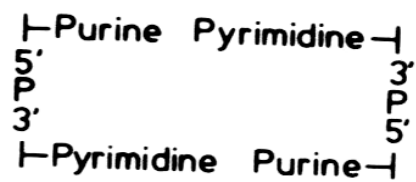
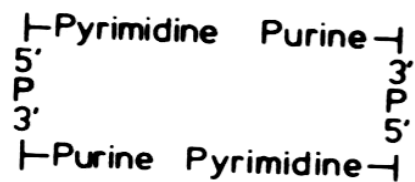


Table 3

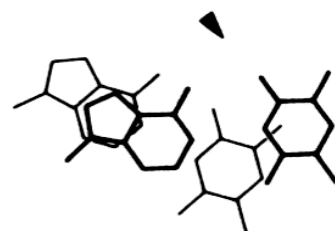
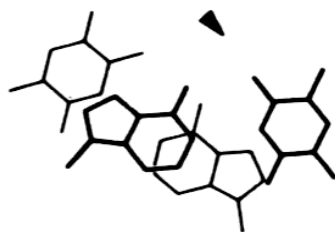
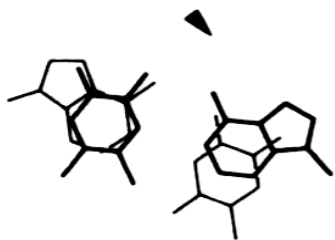
Total Stacking Energies [kcal/
mole dimer] for the Ten Possible Dimers
in B-DNA Type Arrangement Obtained
by Quantum Chemical Calculations^a
[From (542)]

Stacked dimers	Stacking energies [kcal/mole dimer]
$\begin{array}{c} \uparrow \text{C} \cdot \text{G} \downarrow \\ \uparrow \text{G} \cdot \text{C} \downarrow \end{array}$	- 14.59
$\begin{array}{c} \uparrow \text{C} \cdot \text{G} \downarrow \\ \uparrow \text{A} \cdot \text{T} \downarrow \end{array} \quad \begin{array}{c} \uparrow \text{T} \cdot \text{A} \downarrow \\ \uparrow \text{G} \cdot \text{C} \downarrow \end{array}$	- 10.51
$\begin{array}{c} \uparrow \text{C} \cdot \text{G} \downarrow \\ \uparrow \text{T} \cdot \text{A} \downarrow \end{array} \quad \begin{array}{c} \uparrow \text{A} \cdot \text{T} \downarrow \\ \uparrow \text{G} \cdot \text{C} \downarrow \end{array}$	- 9.81
$\begin{array}{c} \uparrow \text{G} \cdot \text{C} \downarrow \\ \uparrow \text{C} \cdot \text{G} \downarrow \end{array}$	- 9.69
$\begin{array}{c} \uparrow \text{G} \cdot \text{C} \downarrow \\ \uparrow \text{G} \cdot \text{C} \downarrow \end{array} \quad \begin{array}{c} \uparrow \text{C} \cdot \text{G} \downarrow \\ \uparrow \text{C} \cdot \text{G} \downarrow \end{array}$	- 8.26
$\begin{array}{c} \uparrow \text{T} \cdot \text{A} \downarrow \\ \uparrow \text{A} \cdot \text{T} \downarrow \end{array}$	- 6.57
$\begin{array}{c} \uparrow \text{G} \cdot \text{C} \downarrow \\ \uparrow \text{T} \cdot \text{A} \downarrow \end{array} \quad \begin{array}{c} \uparrow \text{A} \cdot \text{T} \downarrow \\ \uparrow \text{C} \cdot \text{G} \downarrow \end{array}$	- 6.57
$\begin{array}{c} \uparrow \text{G} \cdot \text{C} \downarrow \\ \uparrow \text{T} \cdot \text{A} \downarrow \end{array} \quad \begin{array}{c} \uparrow \text{T} \cdot \text{A} \downarrow \\ \uparrow \text{C} \cdot \text{G} \downarrow \end{array}$	- 6.78
$\begin{array}{c} \uparrow \text{A} \cdot \text{T} \downarrow \\ \uparrow \text{A} \cdot \text{T} \downarrow \end{array} \quad \begin{array}{c} \uparrow \text{T} \cdot \text{A} \downarrow \\ \uparrow \text{T} \cdot \text{A} \downarrow \end{array}$	- 5.37
$\begin{array}{c} \uparrow \text{A} \cdot \text{T} \downarrow \\ \uparrow \text{T} \cdot \text{A} \downarrow \end{array}$	- 3.82

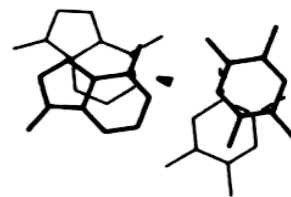
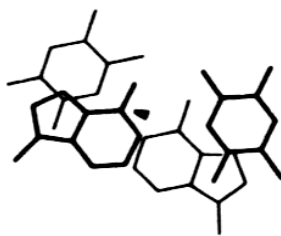
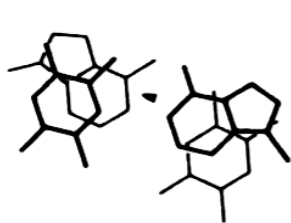
^a Arrows designate direction of sugar-phosphate chain and point from C_{3'} of one sugar unit to C_{5'} of the next, both carbons attached to the same phosphodiester link.



A



B



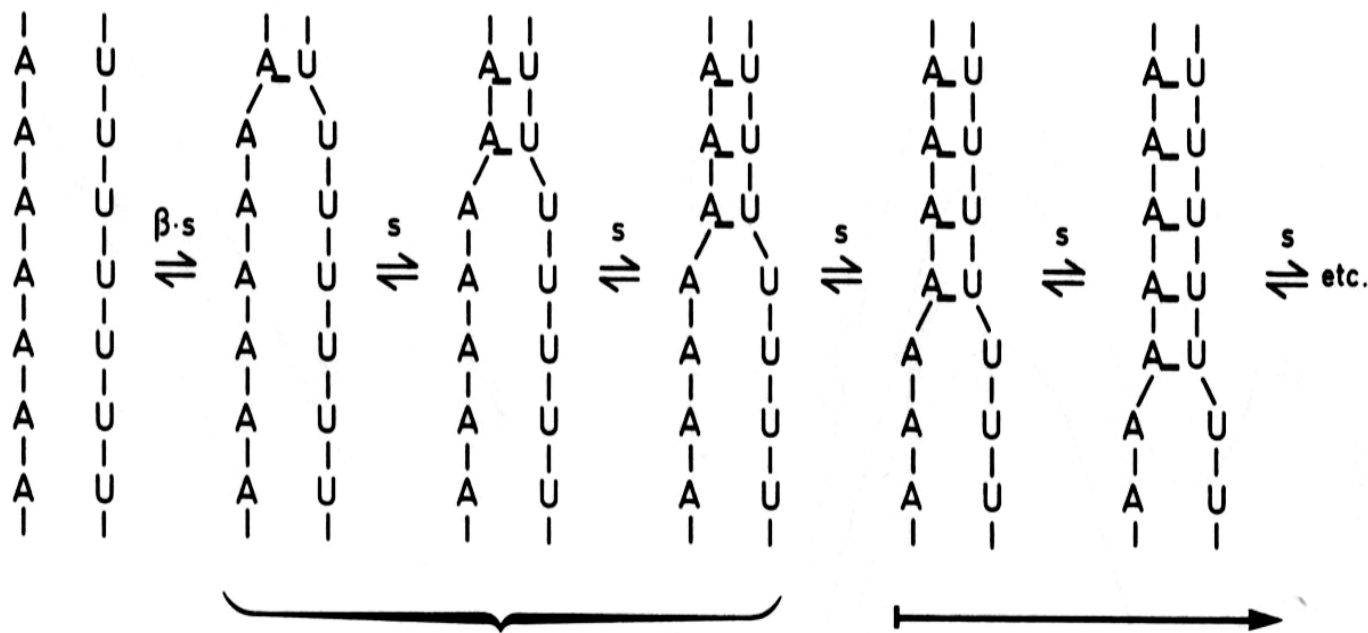


Figure 18

Schematic description of double-helix formation in the case of oligo(A)·oligo(U). In this system, helix growth parameter s is about 10 at 0°C and 1 at the melting temperature. Nucleation parameter β , 10^{-3} liters/mole, diminishes stability constant $K = \beta \cdot s$ of primary base-pair formation but does not influence formation of additional, stacked base-pairs which form cooperatively with $K = s$ according to a *linear Ising model*. In contrast to the *isodesmic model* for base stacking (Figure 6-9), where each step is independent of the other, in the *cooperative process* described by the Ising model, base-pair formation and stacking are influenced by the next neighbors, except for the very first base–base association.

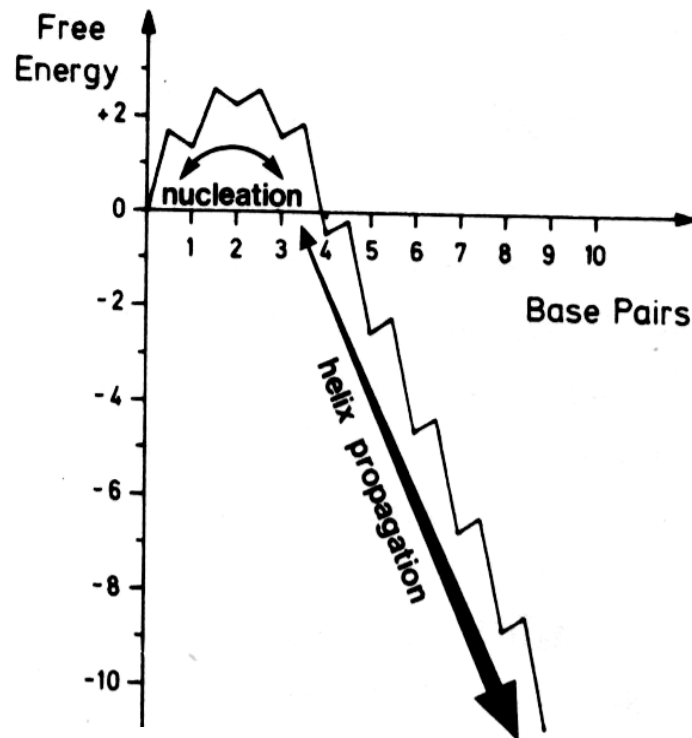


Figure 19

After the unfavorable positive free energy contribution in the nucleation process is overcome, the free energy for additional steps becomes negative and the helix grows spontaneously. Relative total free energy (ΔG) of helix formation in arbitrary units is plotted as a function of the number of consecutive, stacked base-pairs assembled into a helical array. From (544).