

Δομική βιολογία

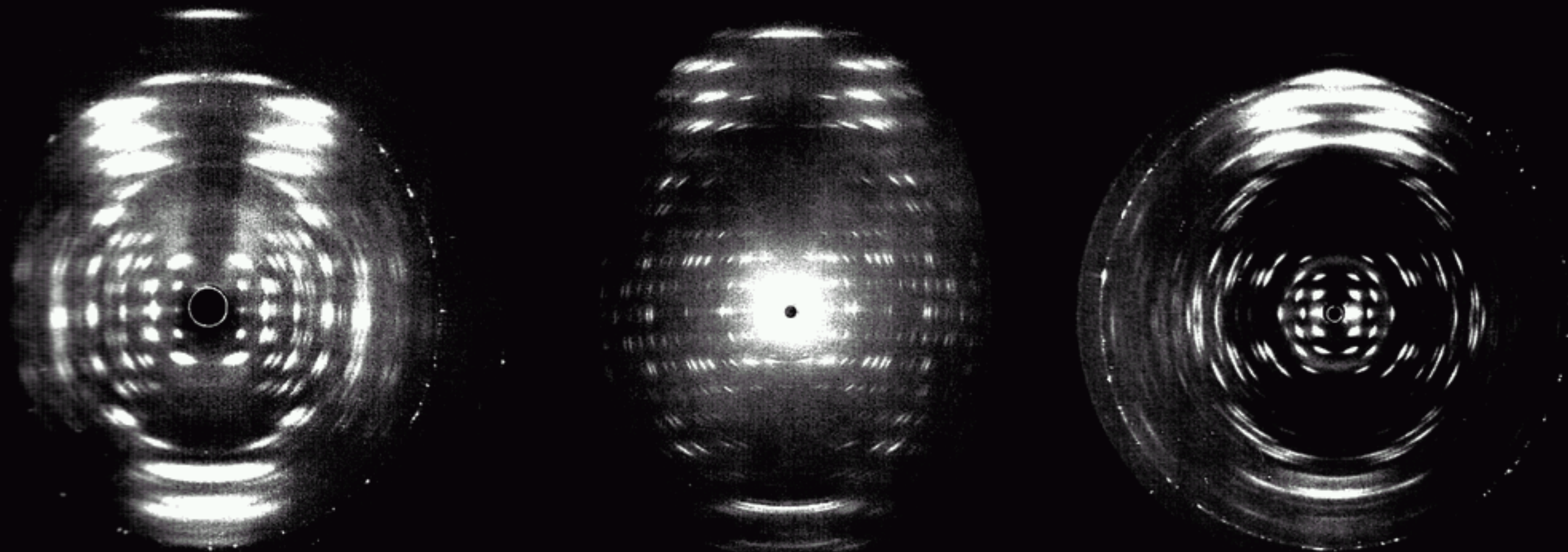
Διάλεξη 10η :

Δομές νουκλεϊκών οξέων.

Προσδιορισμός δομών

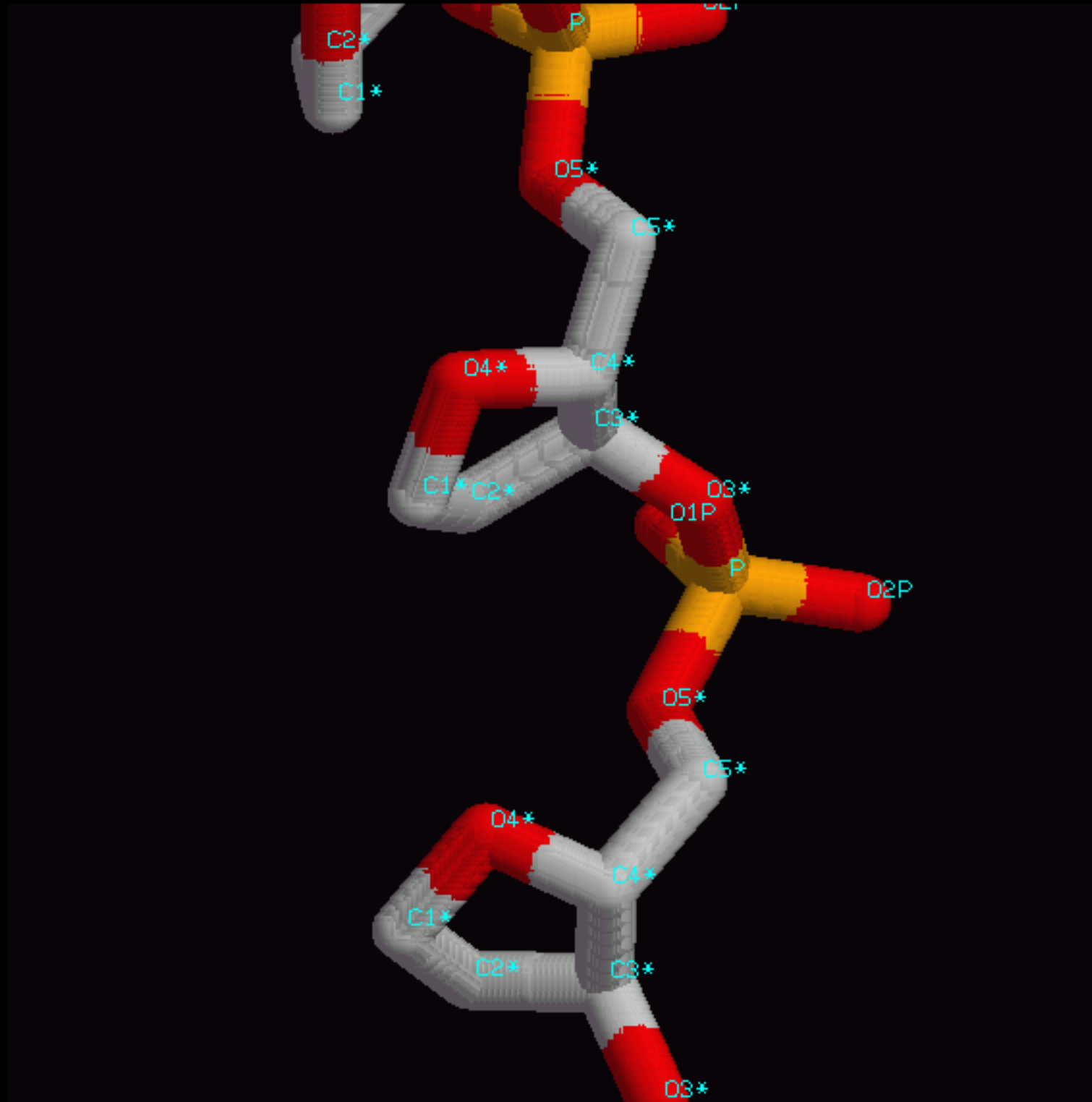
Fiber diffraction

Η ιστορικά (αλλά και ουσιαστικά) πλέον δημοφιλής μέθοδος είναι περίθλαση από παράλληλα διευθετημένες ίνες (fiber diffraction). Από τη δεκαετία του '80 και μετά κυρίως περίθλαση από κρυστάλλους και NMR.



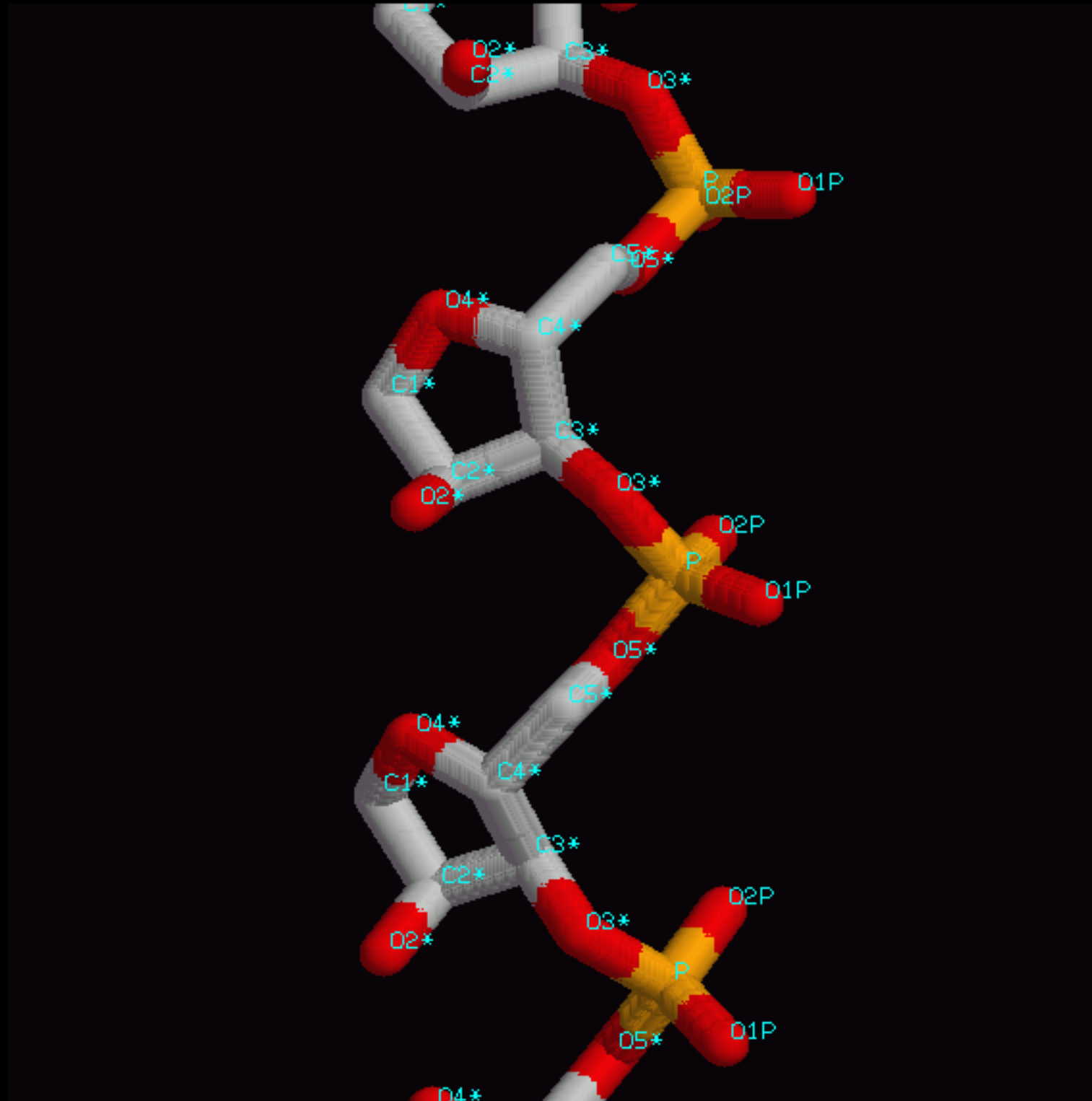
Φωσφοδιεστερικός σκελετός

C2'-endo (DNA)



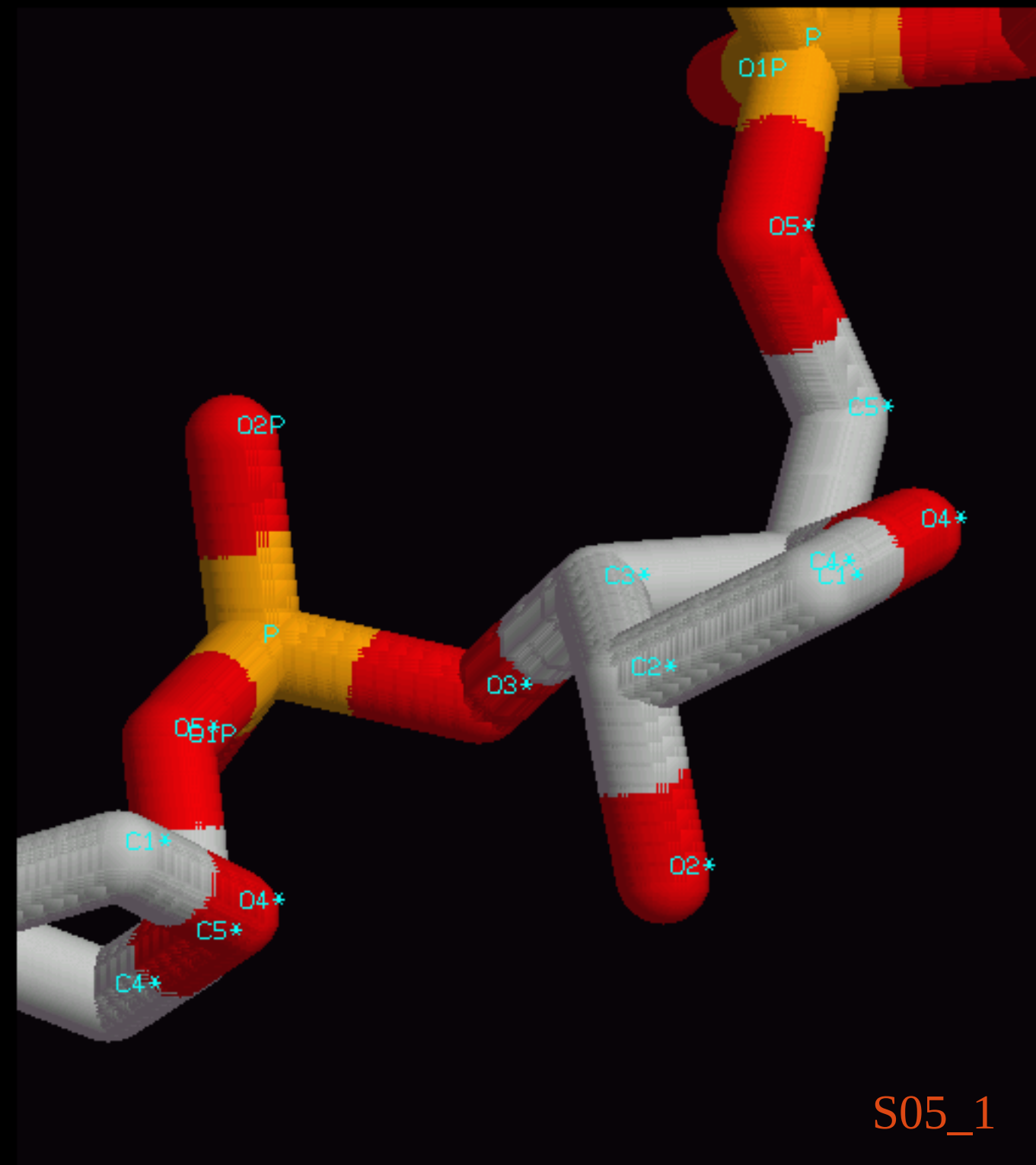
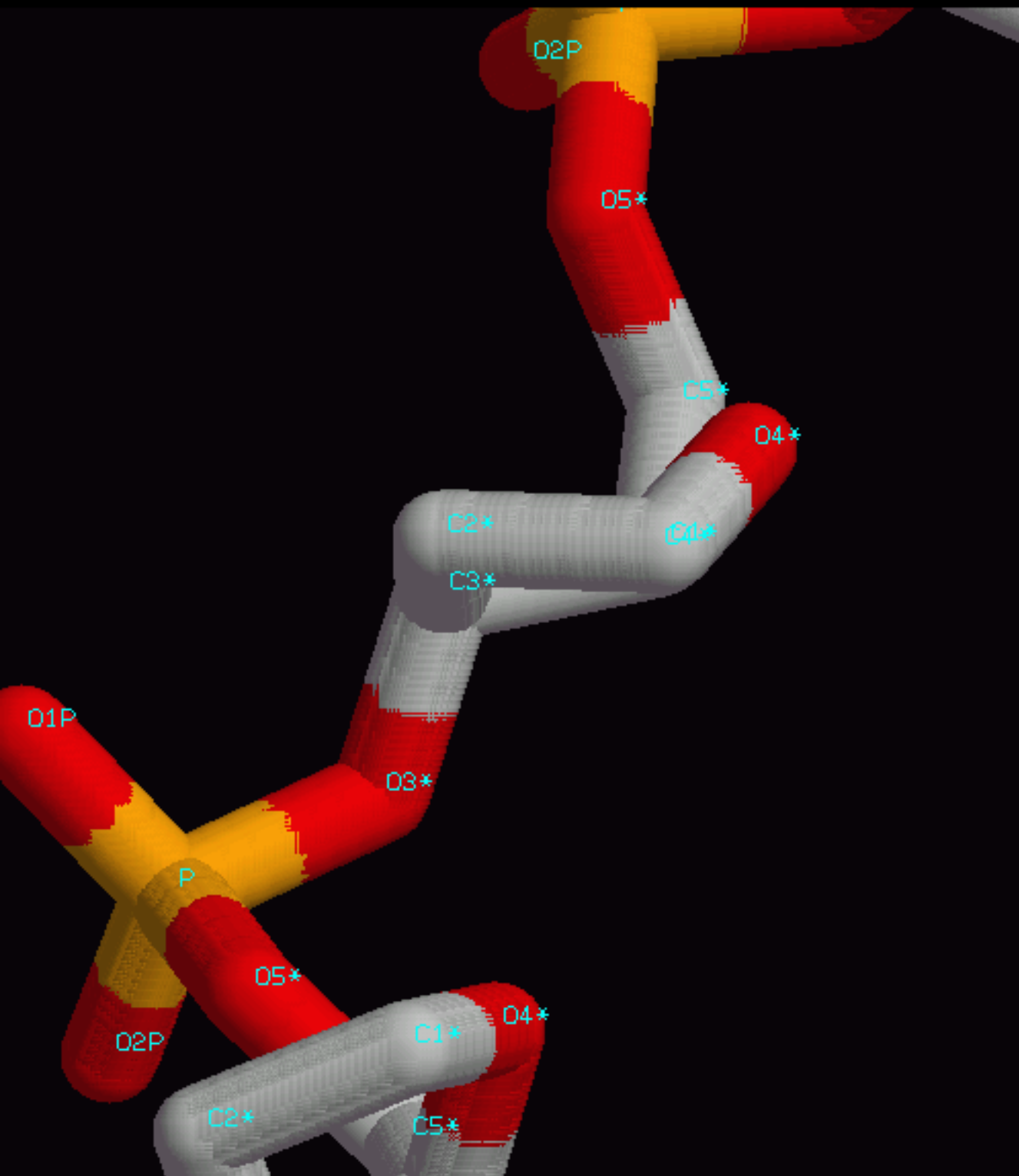
Φωσφοδιεστερικός σκελετός

C3'-endo (RNA)



Φωσφοδιεστερικός σκελετός

C2'-endo vs. C3'-endo furanose rings

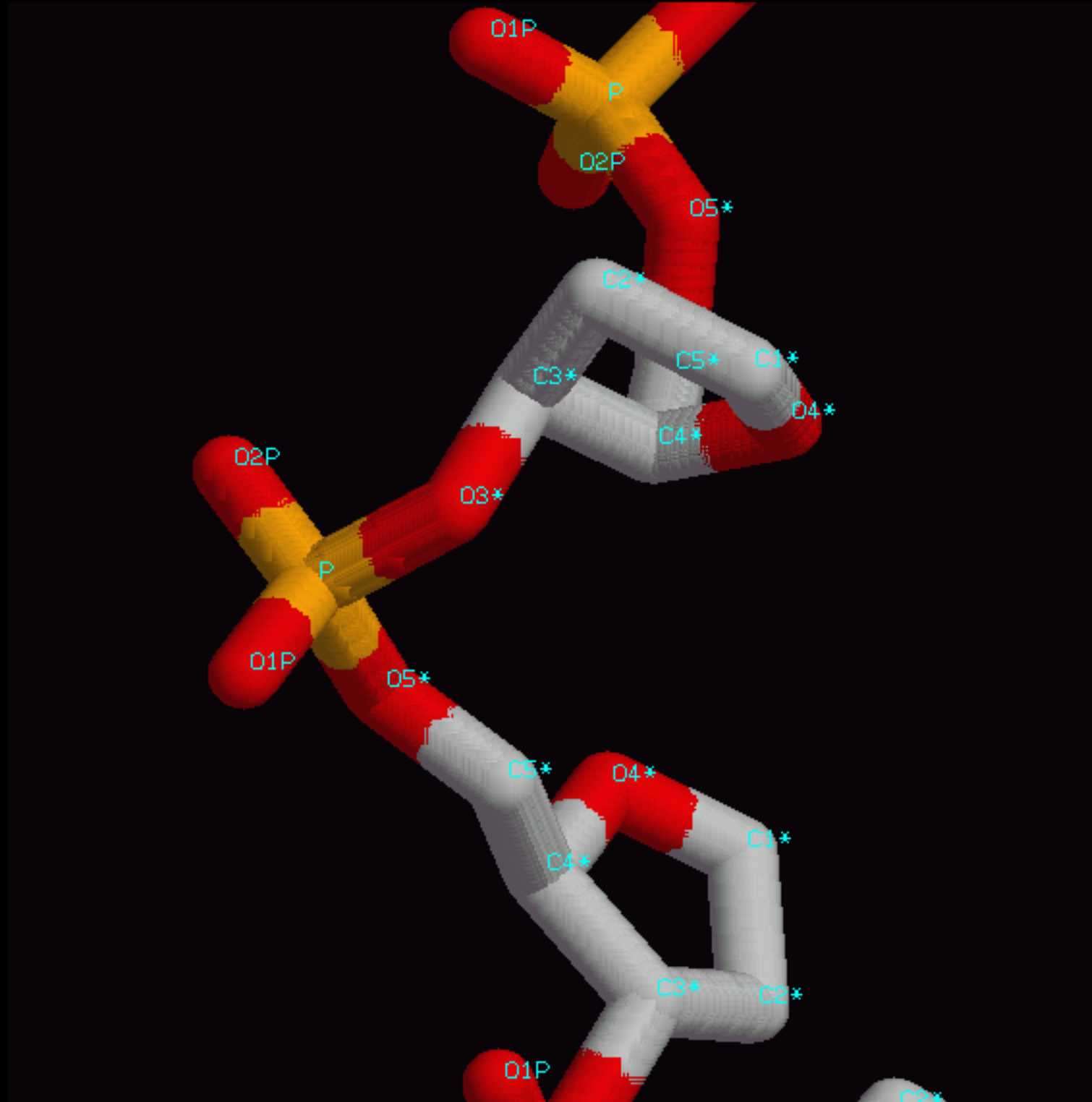


S05_1

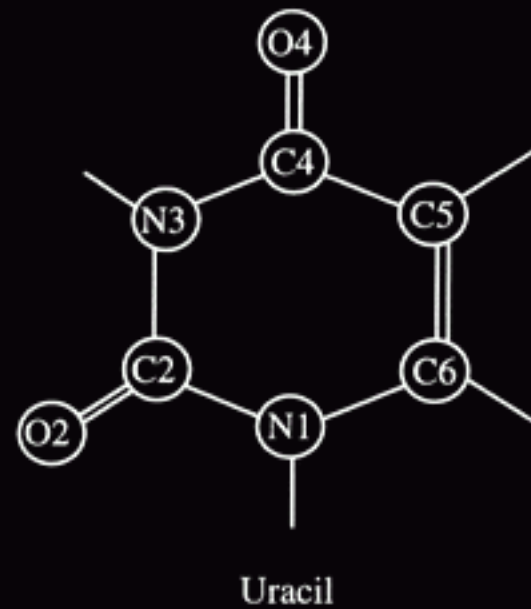
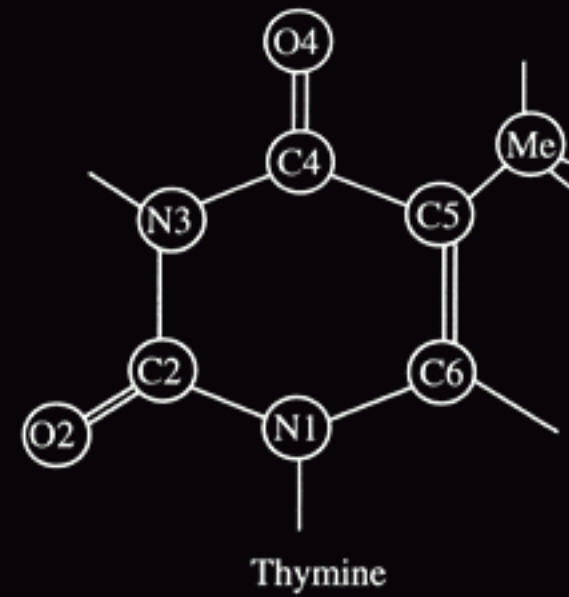
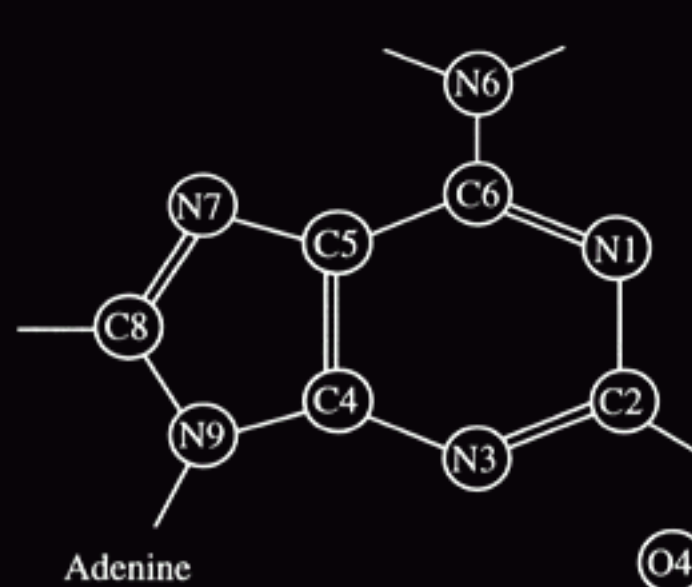
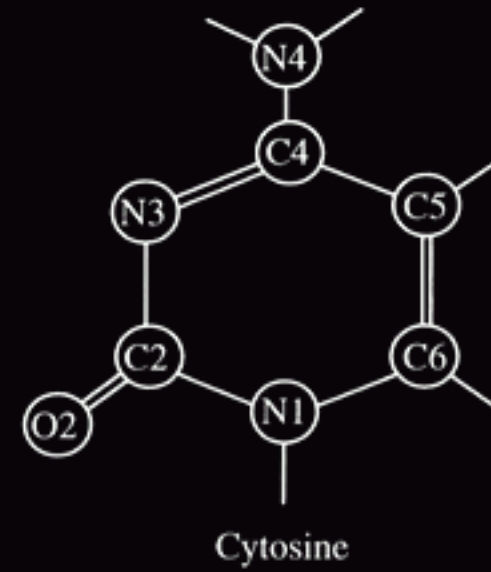
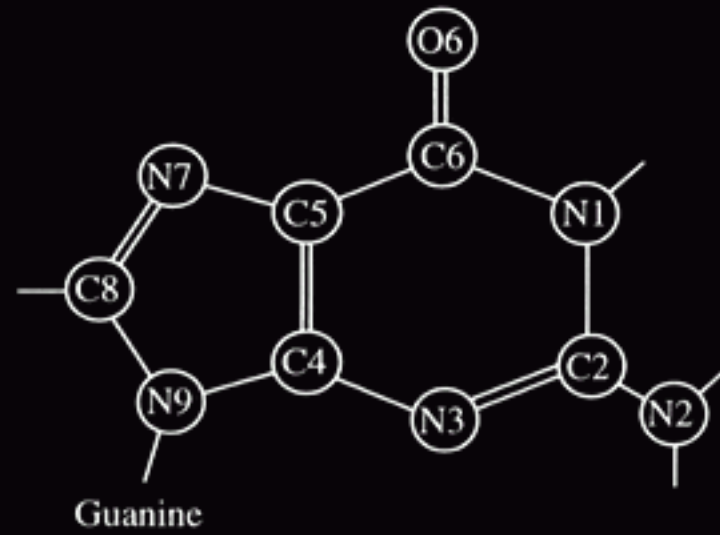
S05_2

Φωσφοδιεστερικός σκελετός

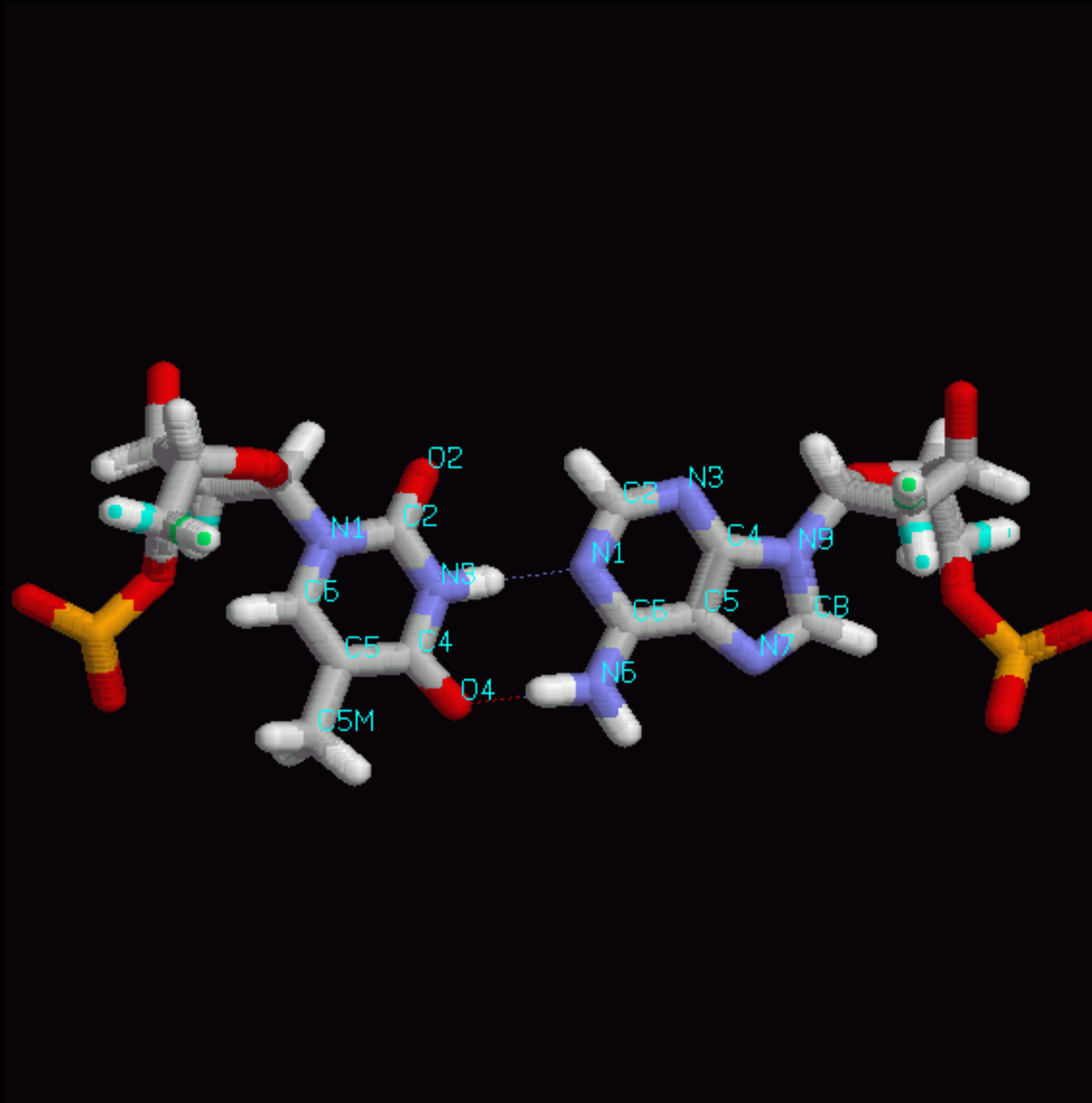
C2'-endo και C3'-endo εναλλάξ (Z-DNA)



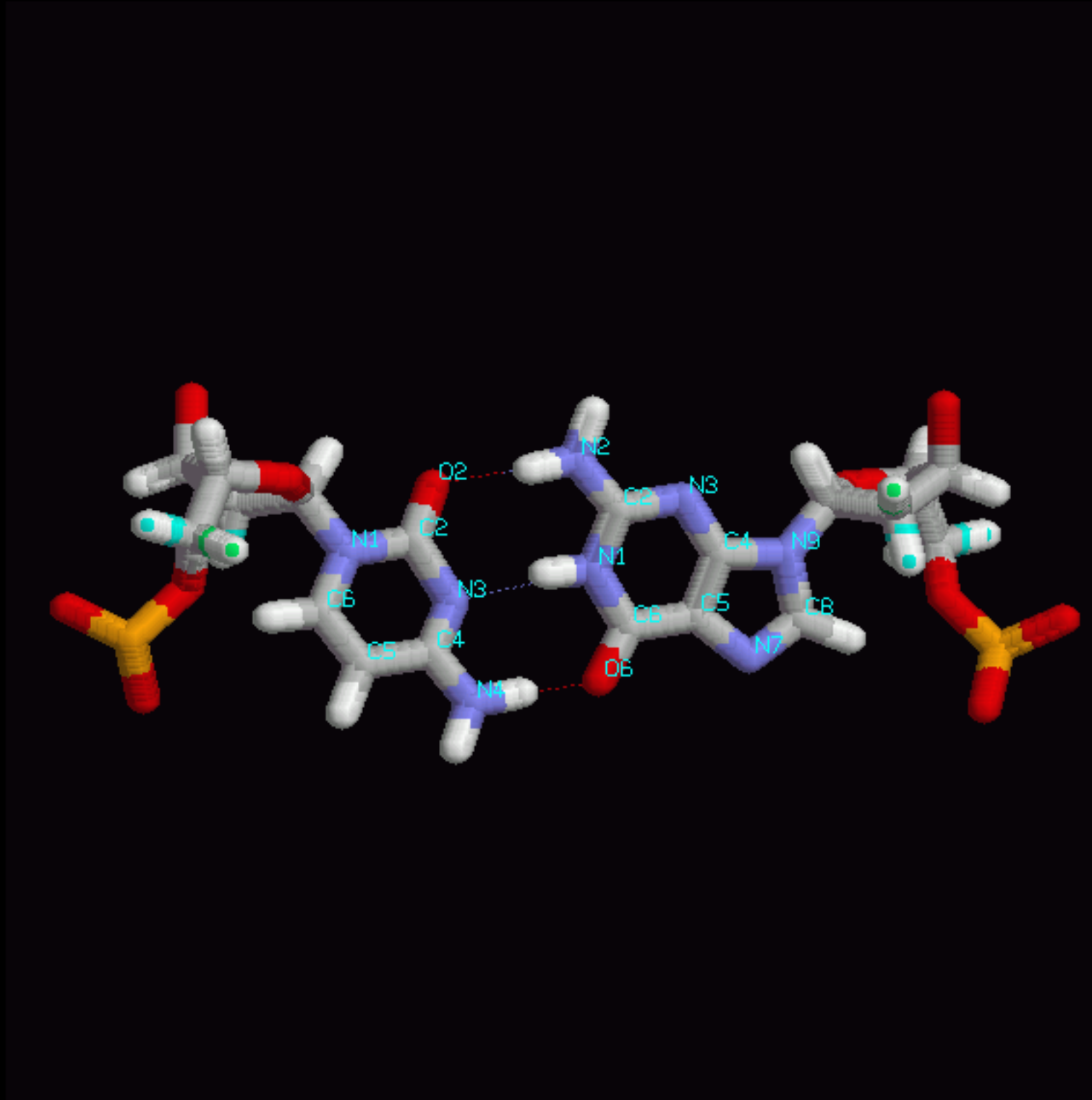
Βάσεις



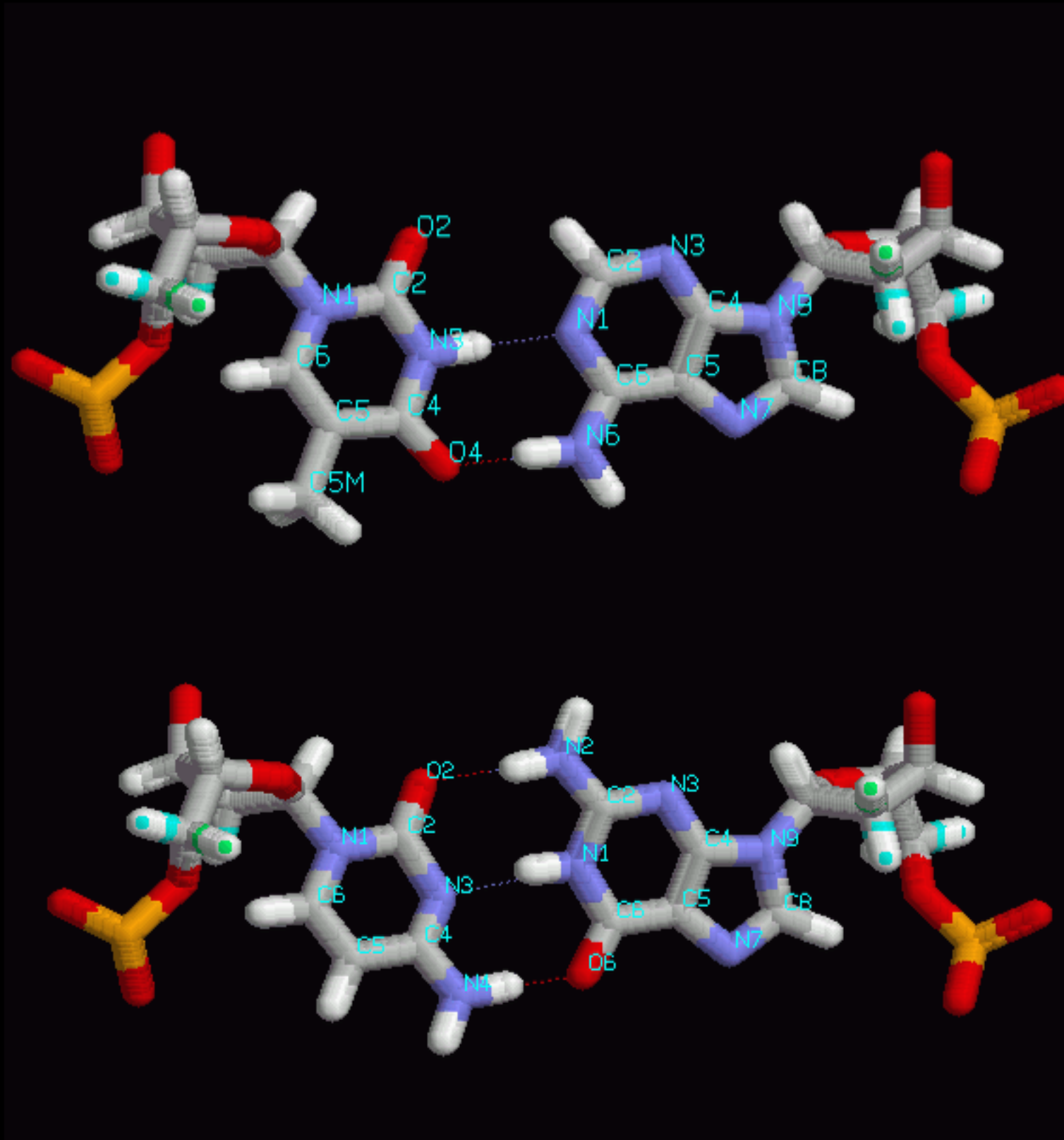
Watson-Crick AT



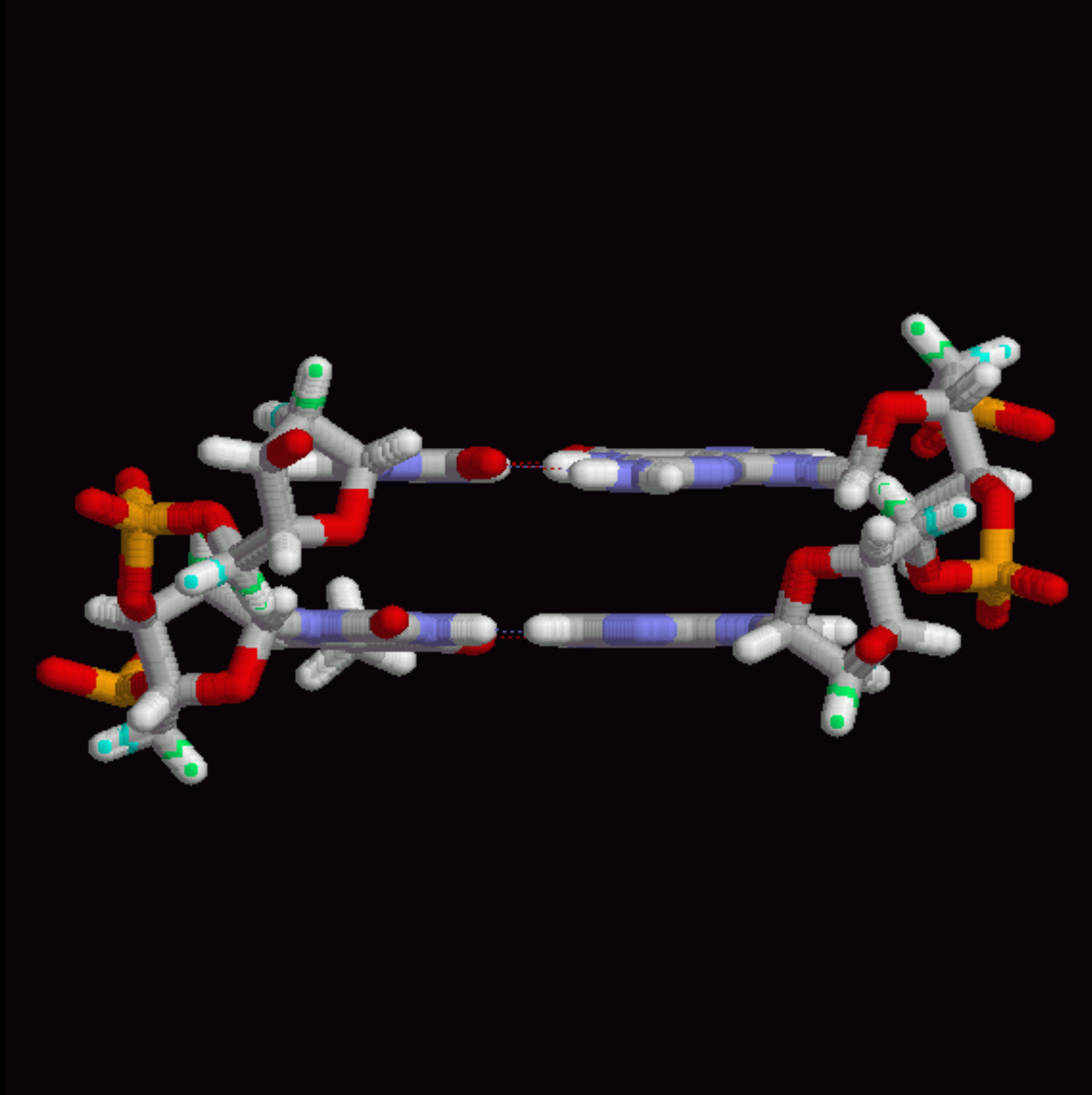
Watson-Crick GC



Watson-Crick AT, GC

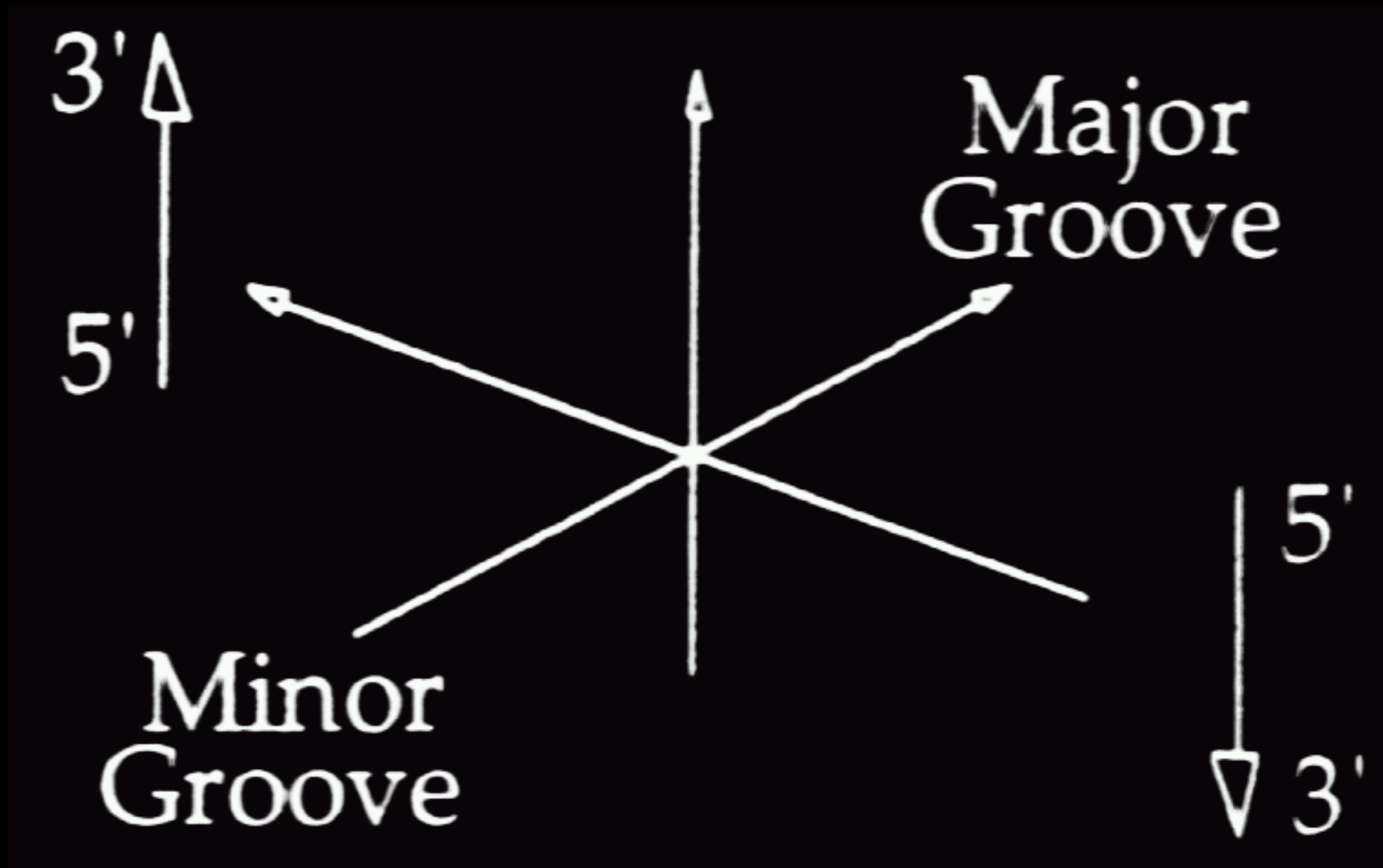


B-DNA, 2 bp, Watson-Crick



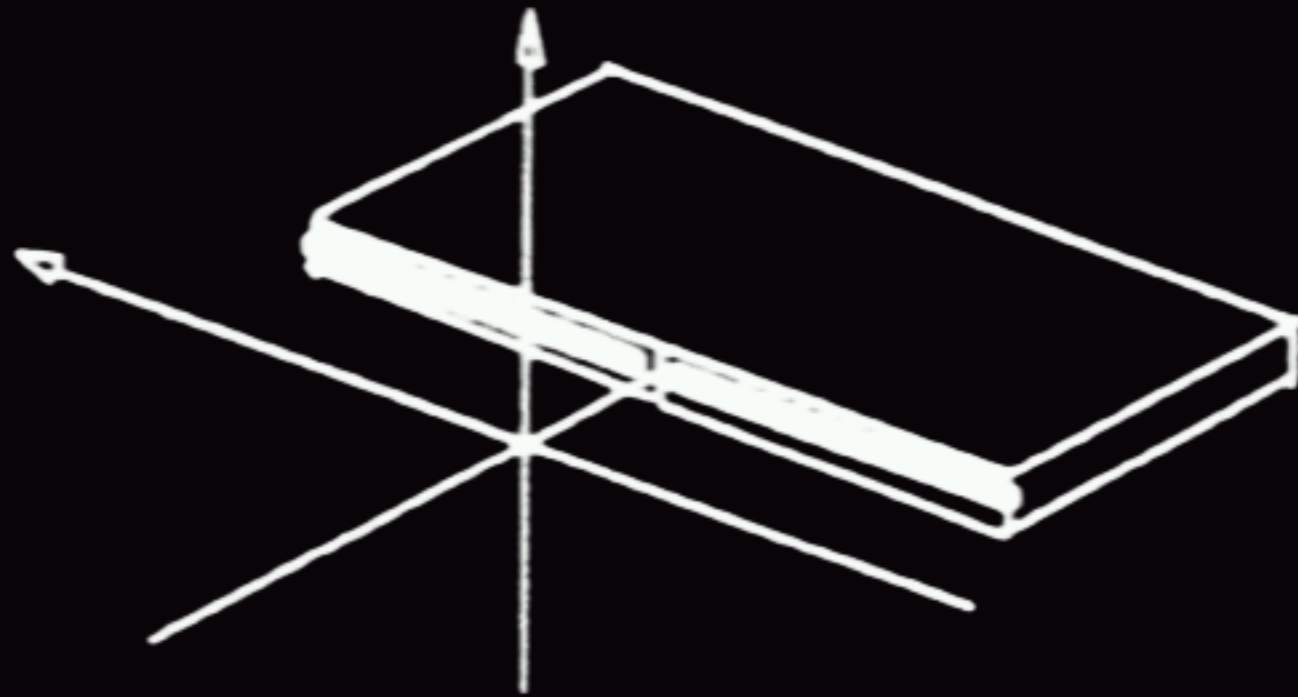
Ελικοειδείς παράμετροι

Πλαίσιο αναφοράς

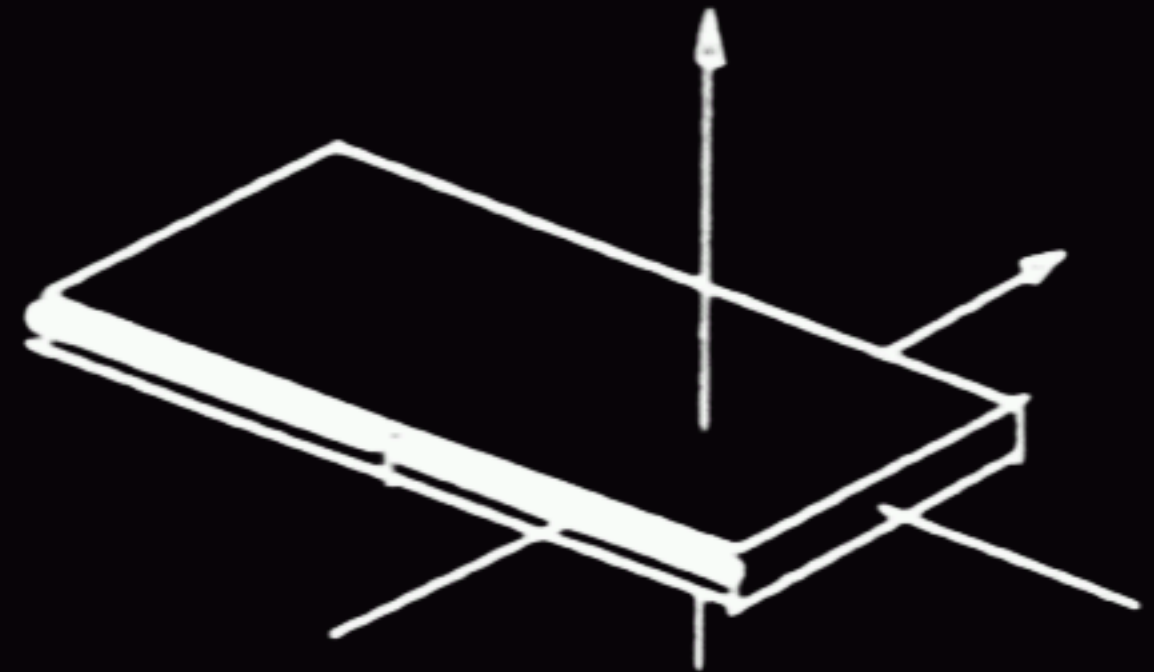


Ελικοειδείς παράμετροι

Μετάθεσης, Base-axis



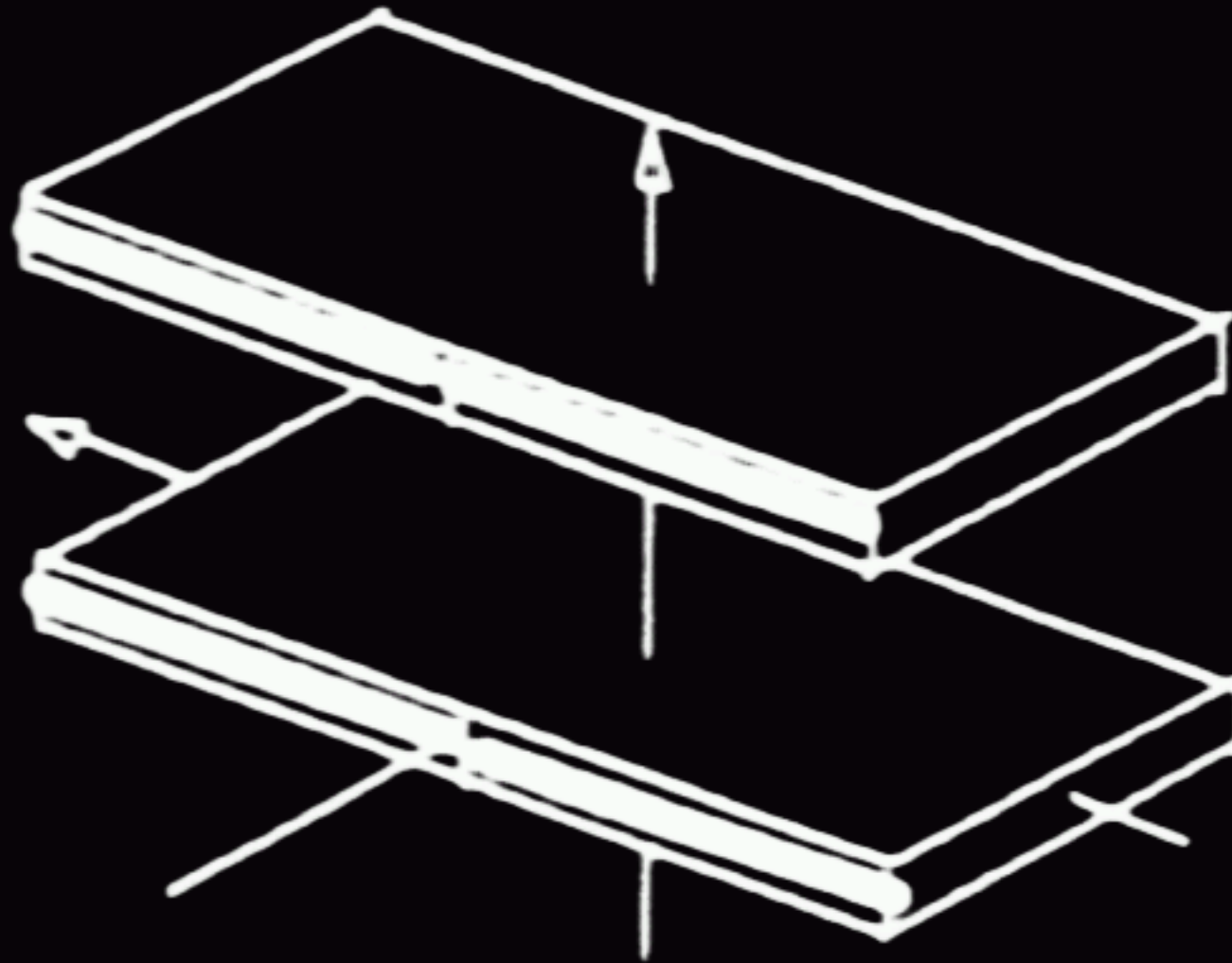
X displacement



Y displacement

Ελικοειδείς παράμετροι

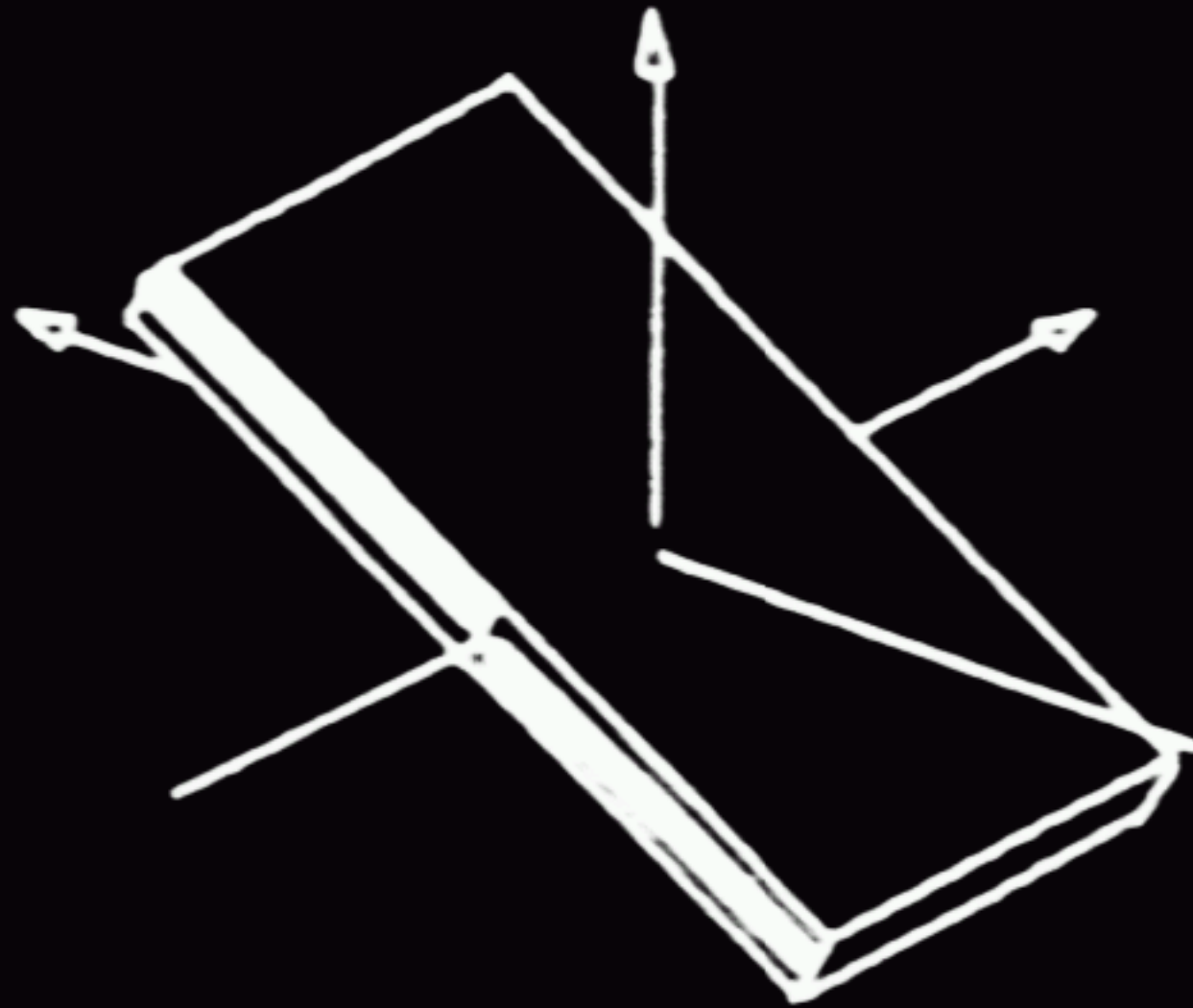
Μετάθεσης, Inter-base



Rise

Ελικοειδείς παράμετροι

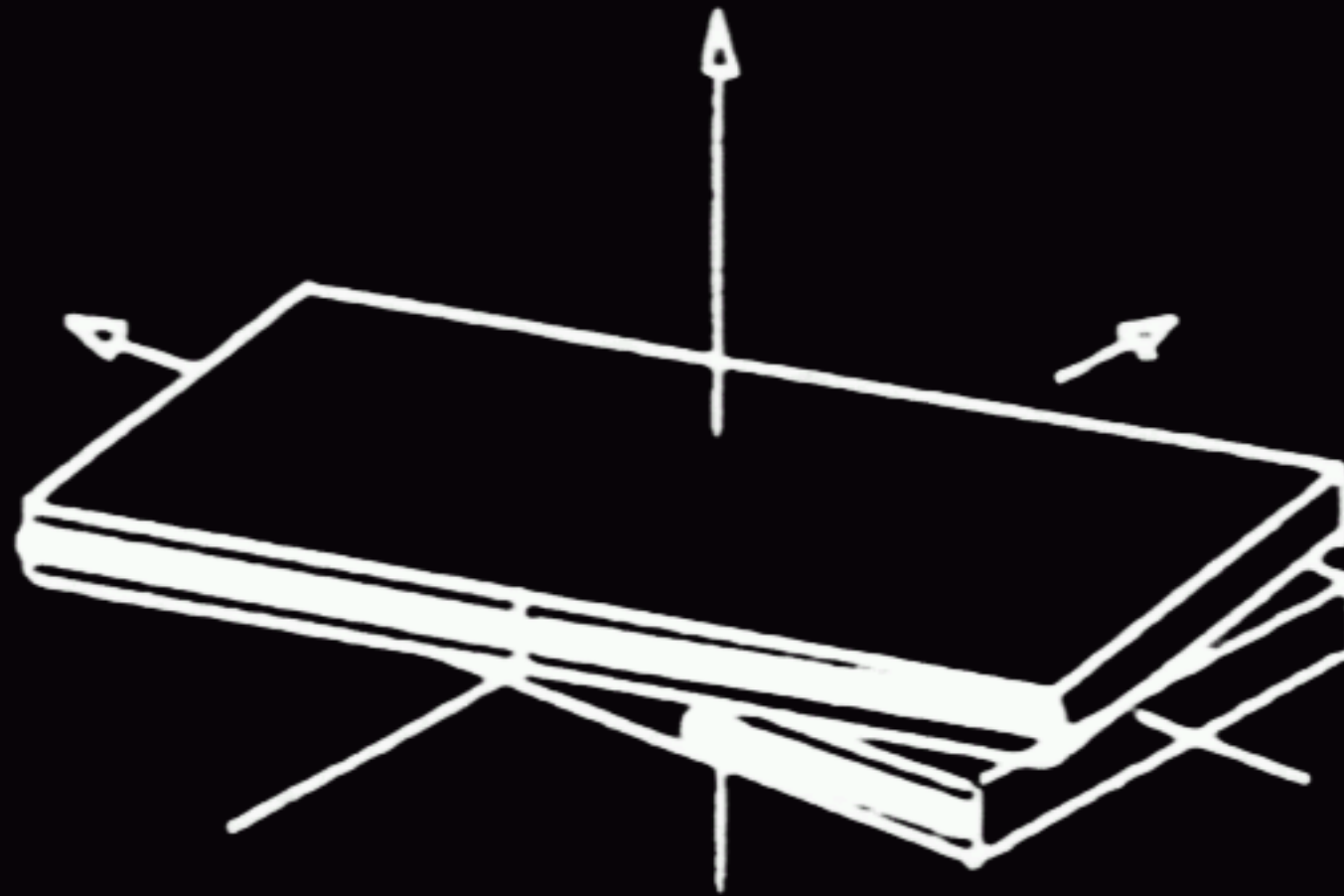
Περιστροφής, Base-axis



Inclination

Ελικοειδείς παράμετροι

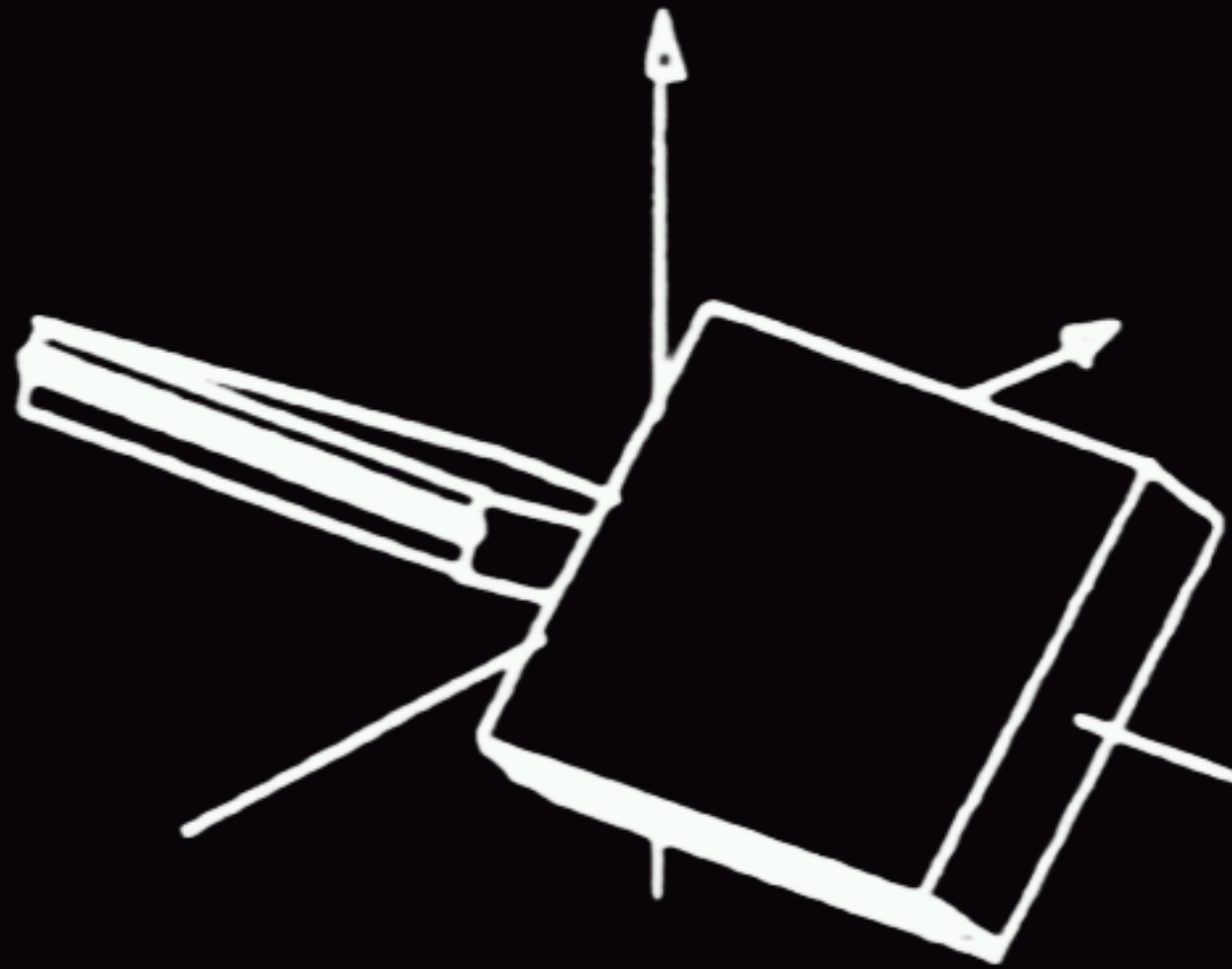
Περιστροφής, Inter-base



Twist

Ελικοειδείς παράμετροι

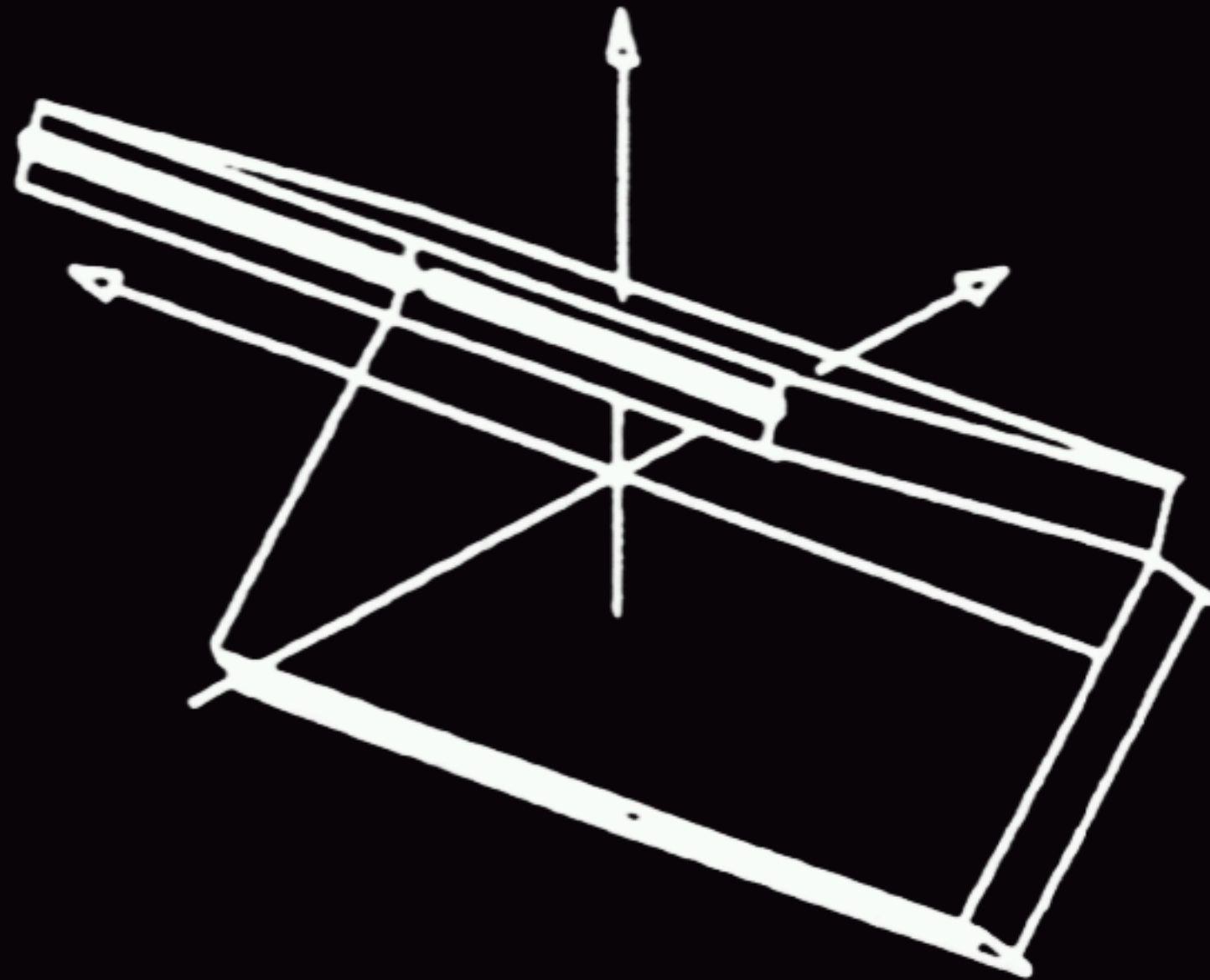
Περιστροφής, Intra-base



Propeller

Ελικοειδείς παράμετροι

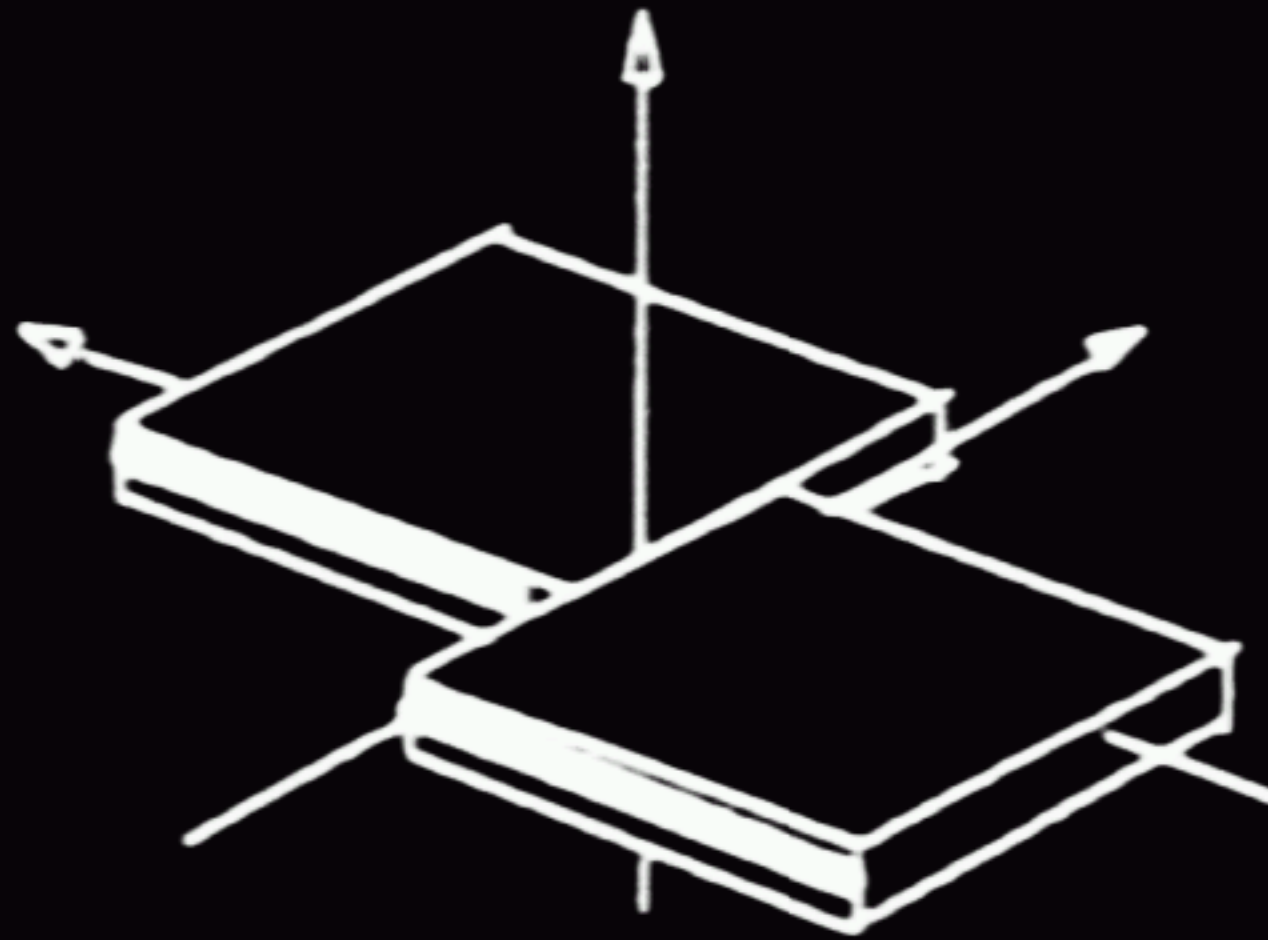
Περιστροφής, Inter-base



Roll

Ελικοειδείς παράμετροι

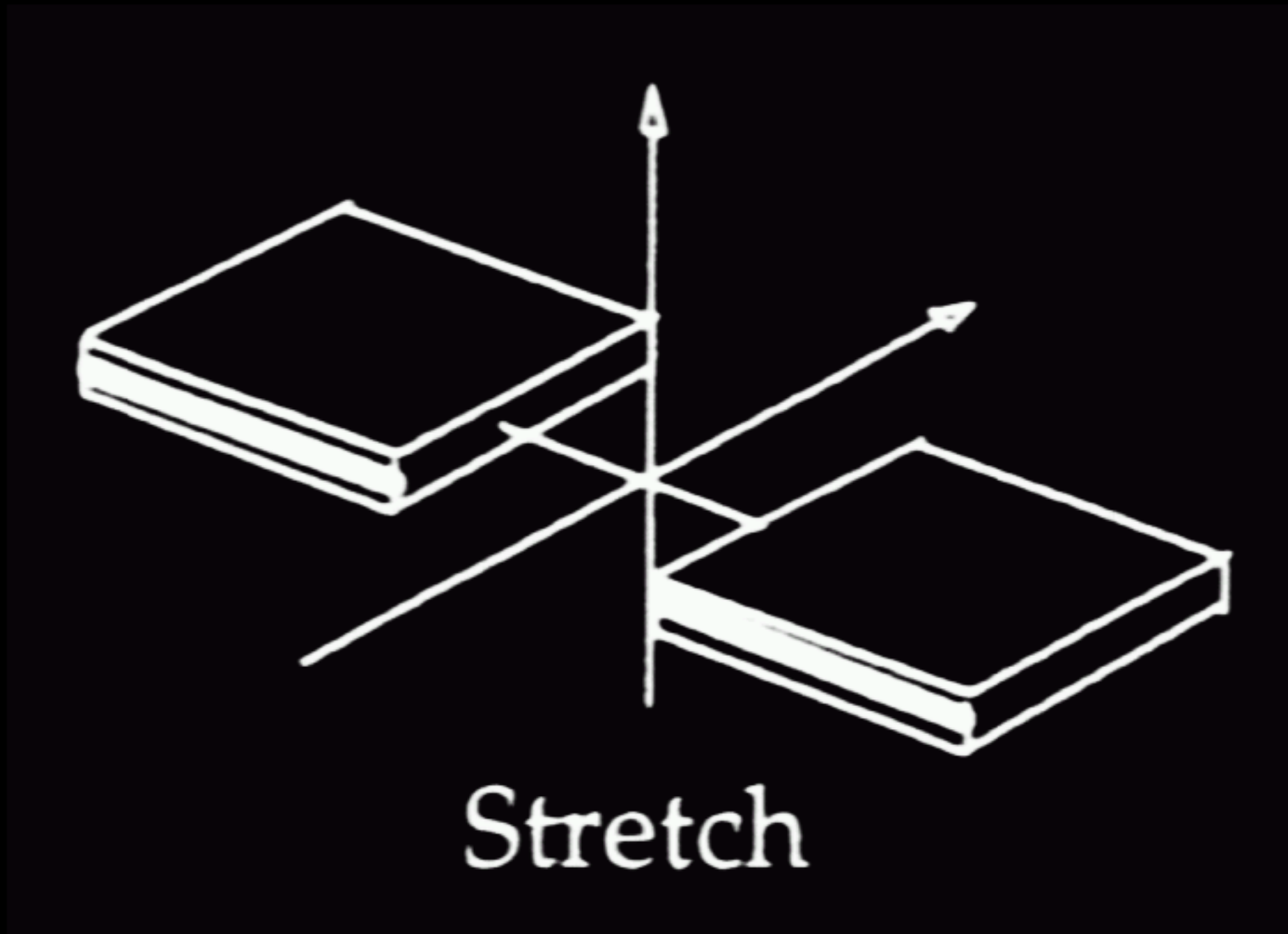
Μετάθεσης, Intra-base



Shear

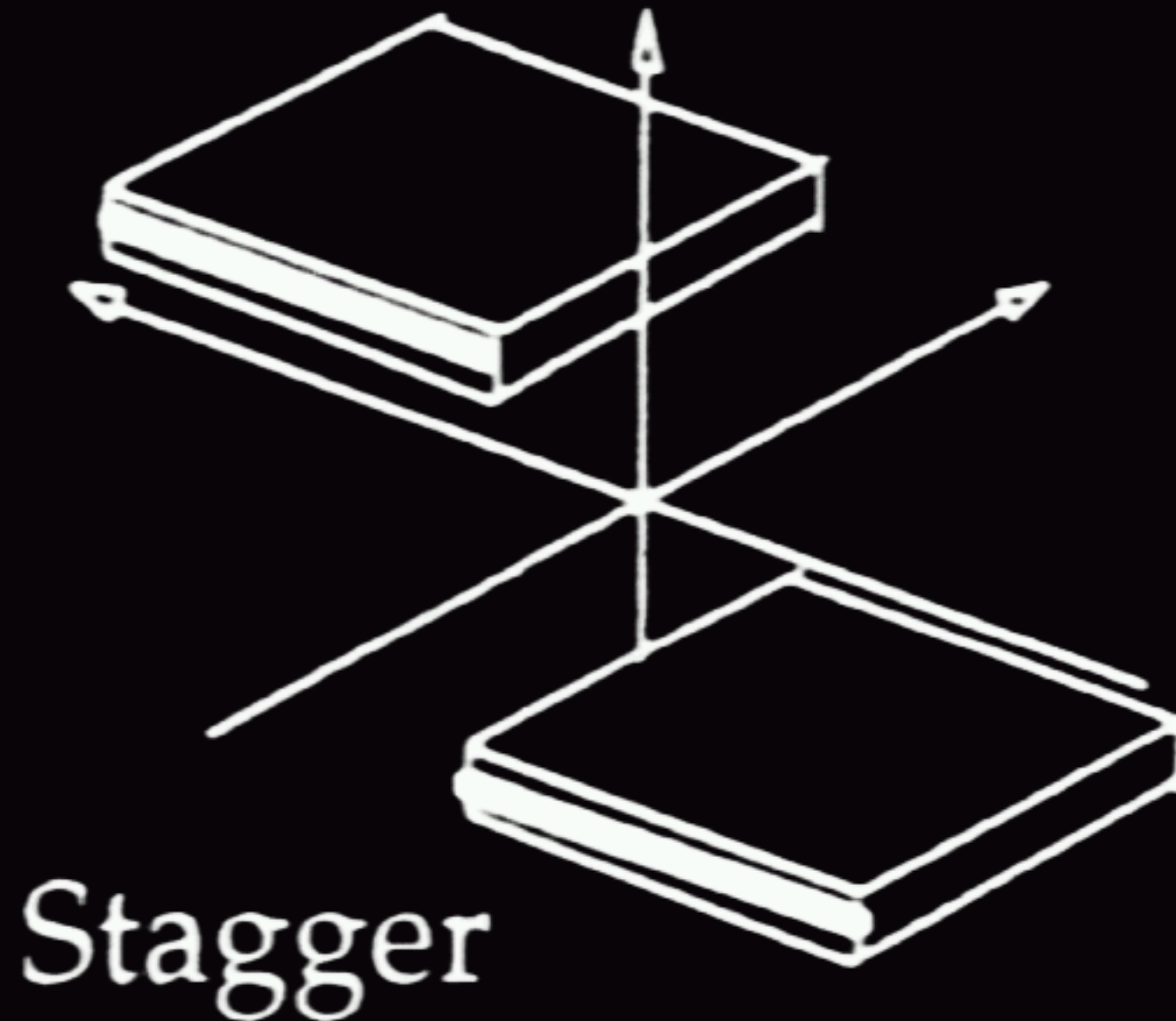
Ελικοειδείς παράμετροι

Μετάθεσης, Intra-base



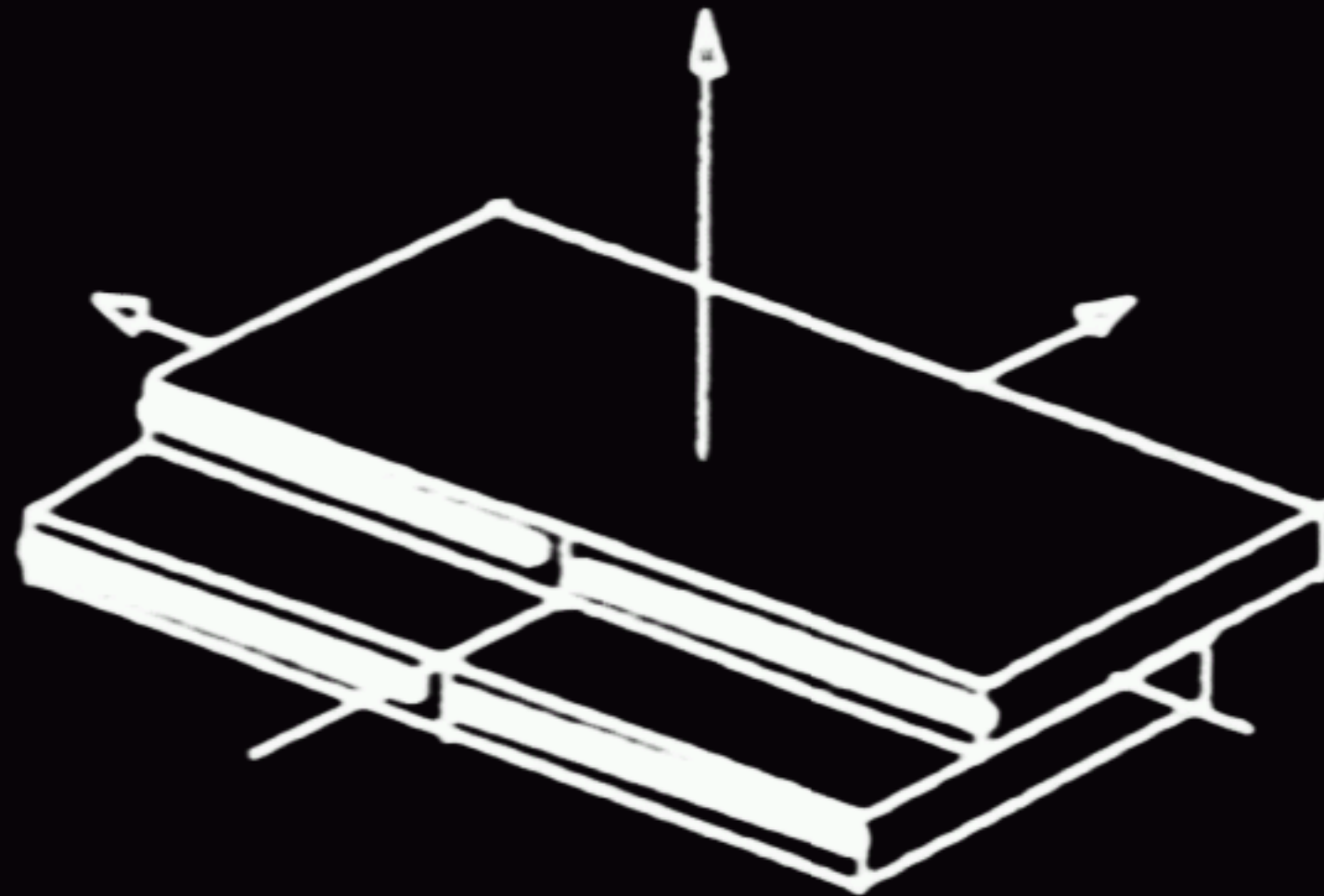
Ελικοειδείς παράμετροι

Μετάθεσης, Intra-base



Ελικοειδείς παράμετροι

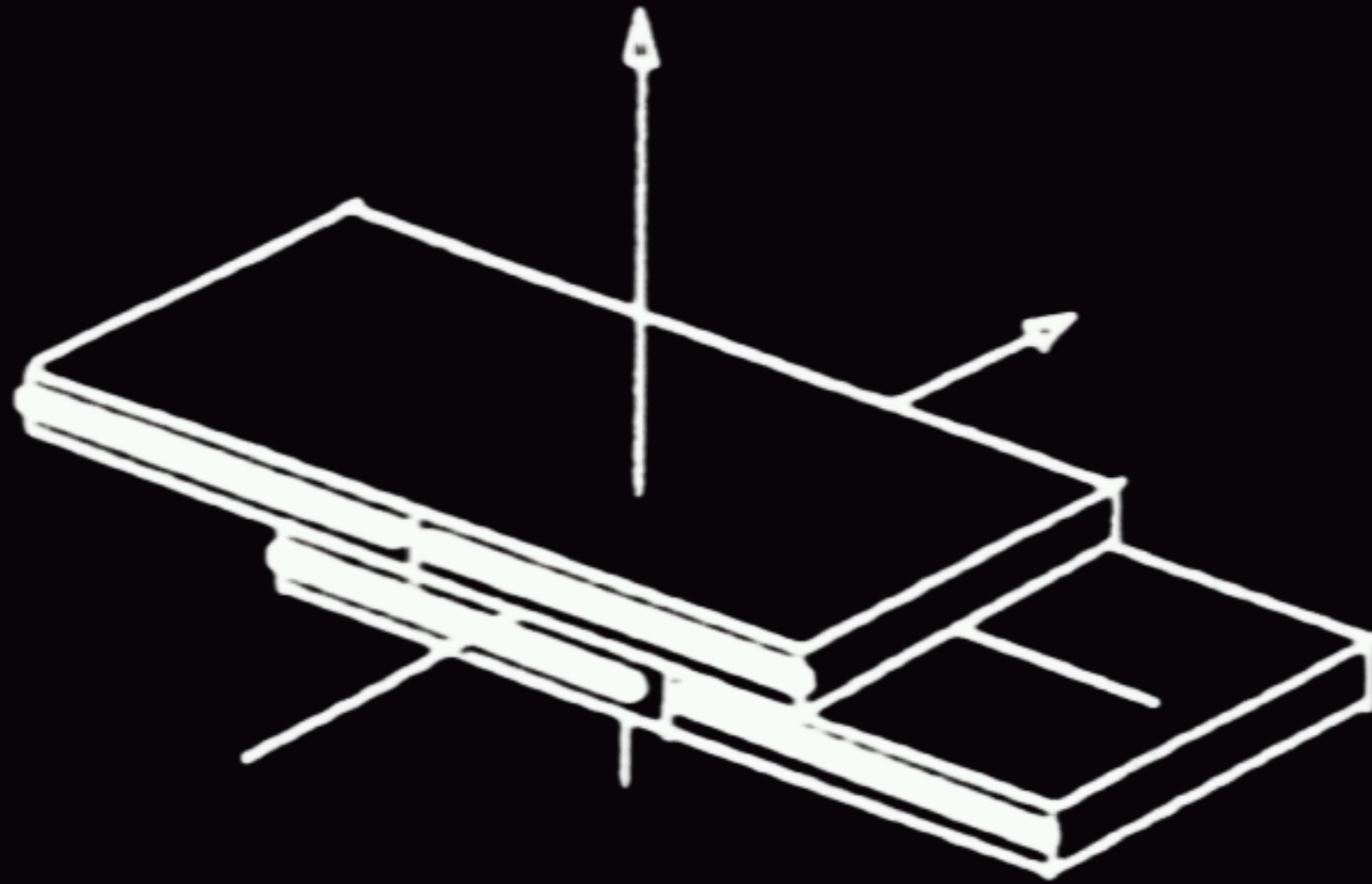
Μετάθεσης, Inter-base



Shift

Ελικοειδείς παράμετροι

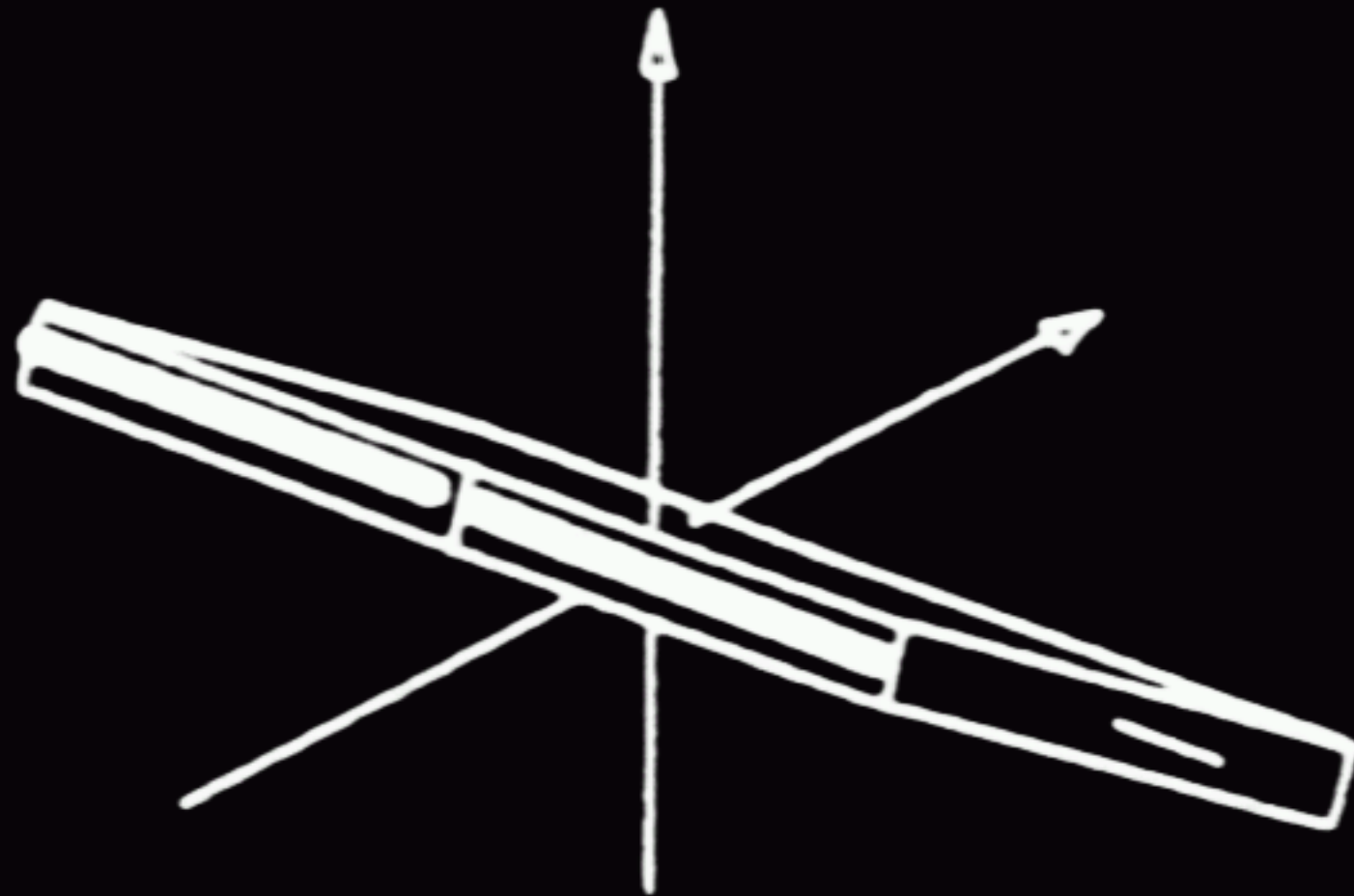
Μετάθεσης, Inter-base



Slide

Ελικοειδείς παράμετροι

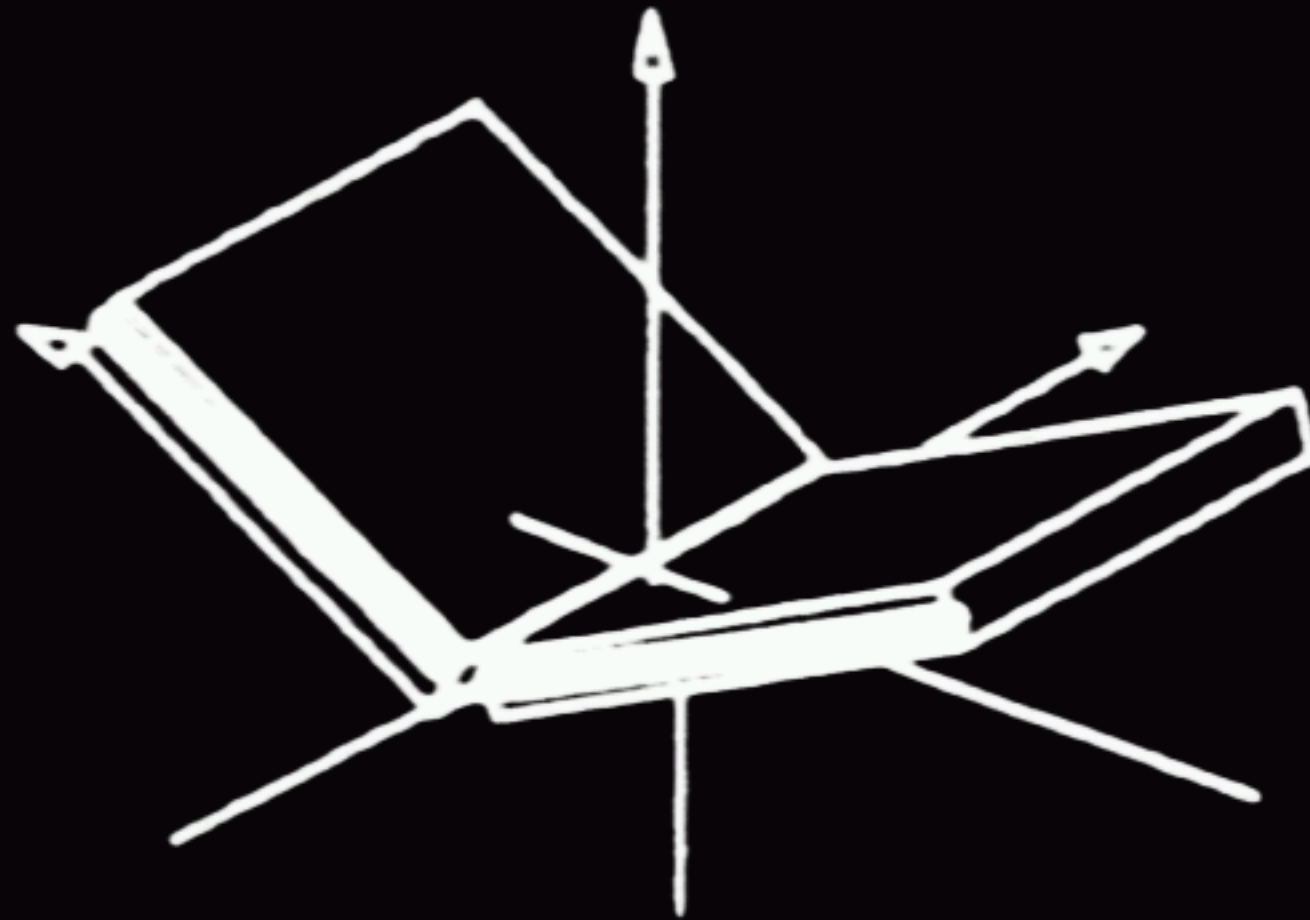
Περιστροφής, Base-axes



Tip

Ελικοειδείς παράμετροι

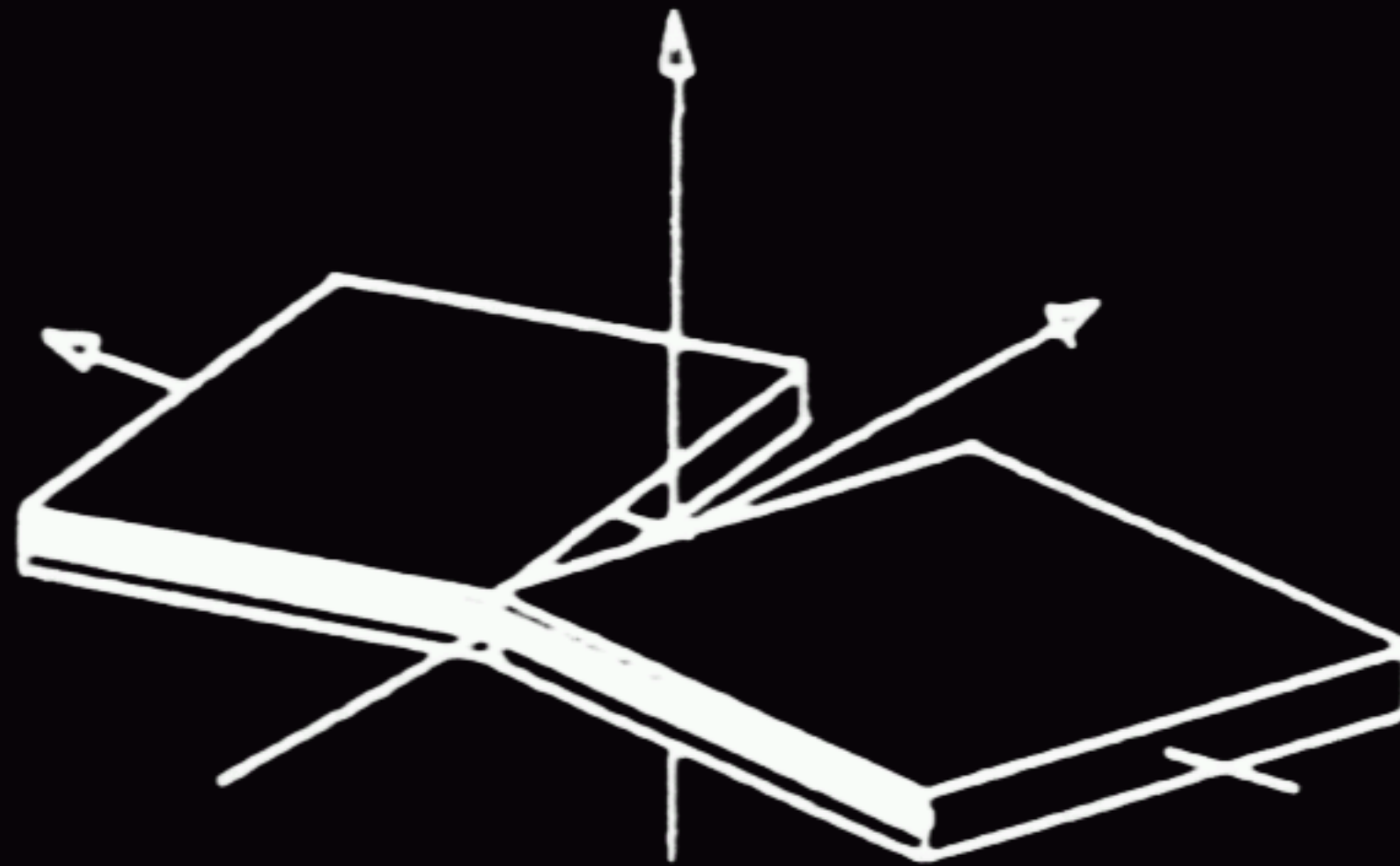
Περιστροφής, Intra-base



Buckle

Ελικοειδείς παράμετροι

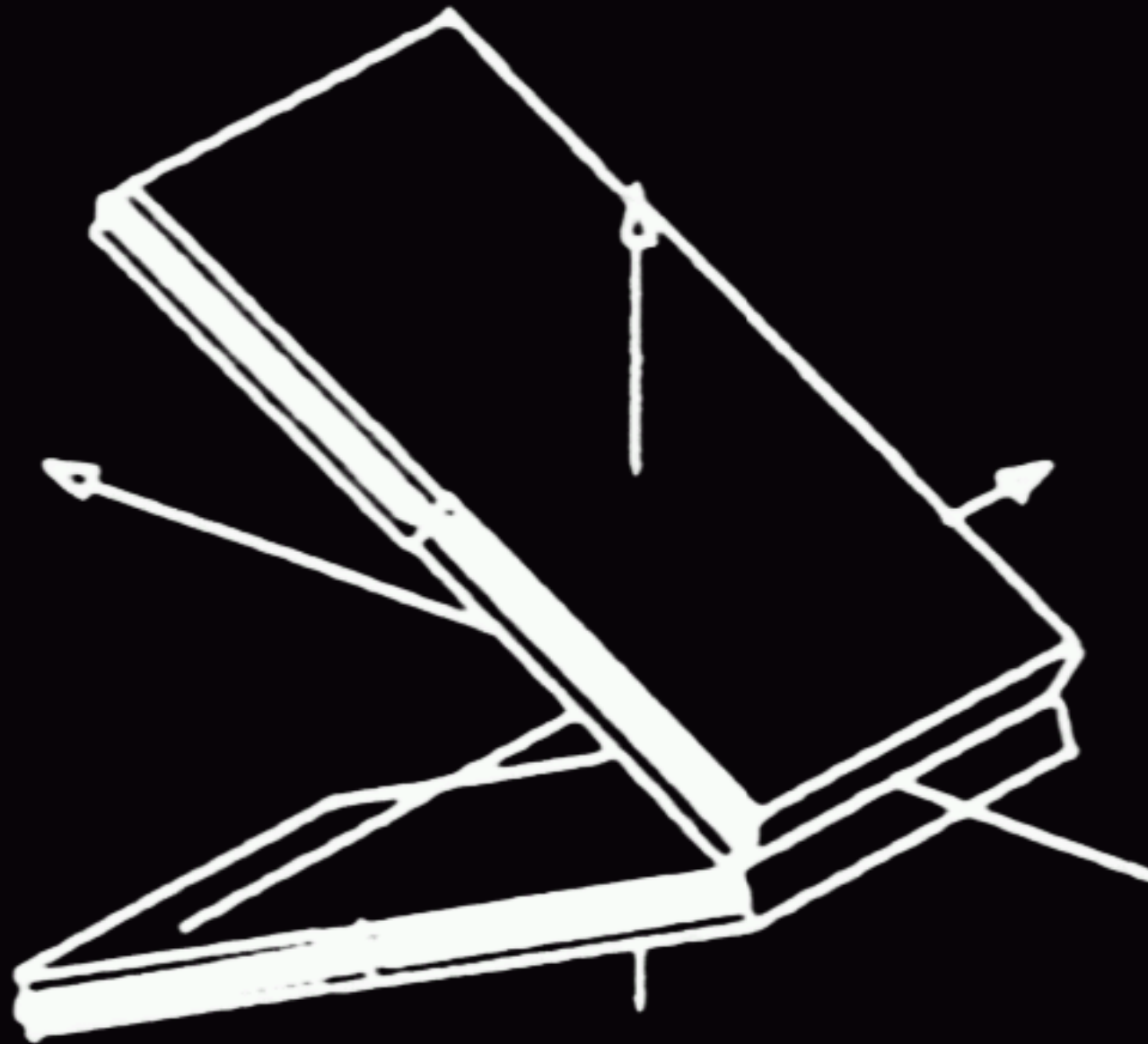
Περιστροφής, Intra-base



Opening

Ελικοειδείς παράμετροι

Περιστροφής, Inter-base



Tilt

B-DNA, Watson-Crick bp



B-DNA

C2'-endo

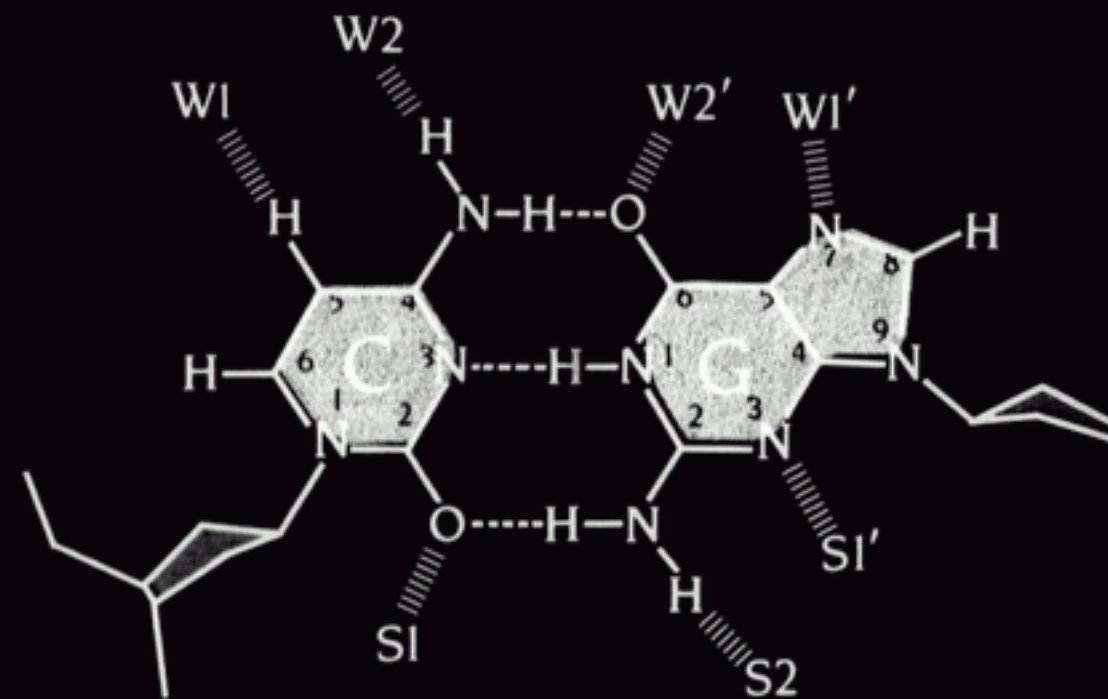
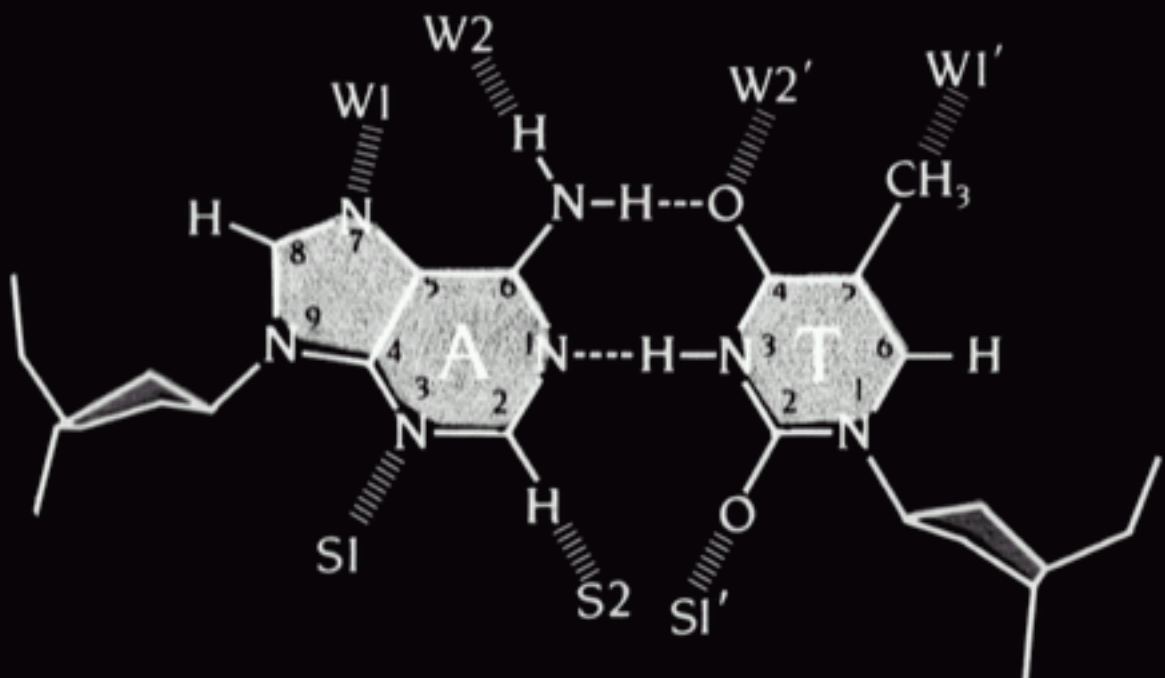
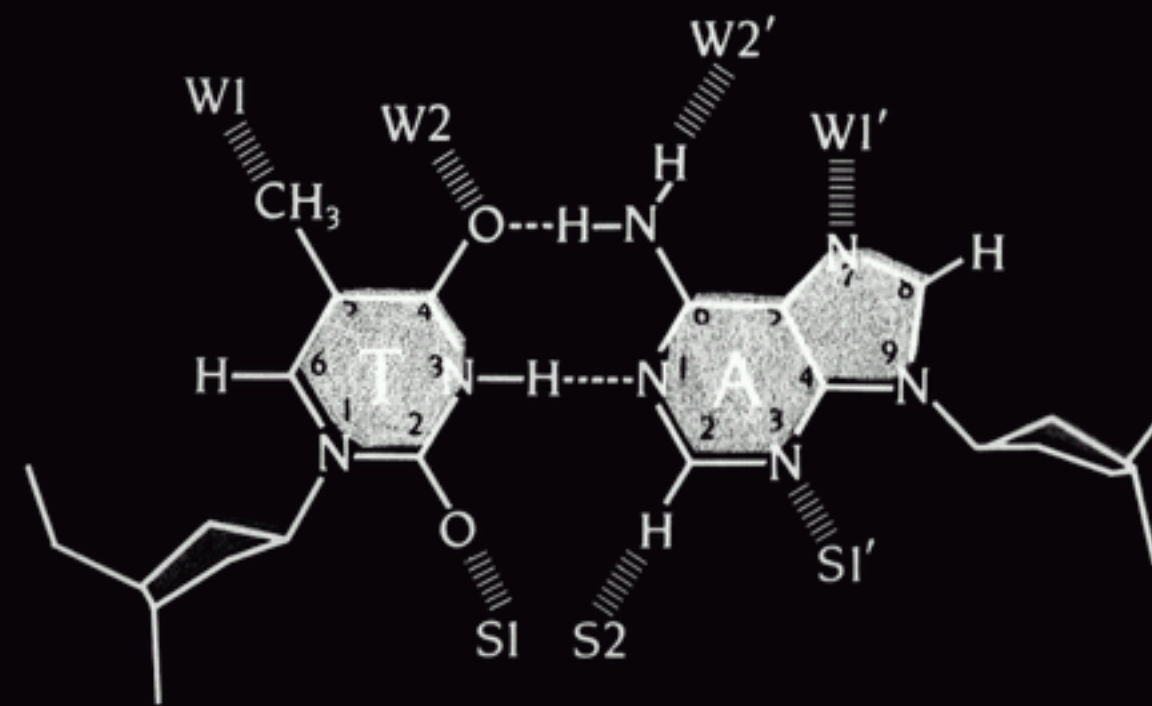
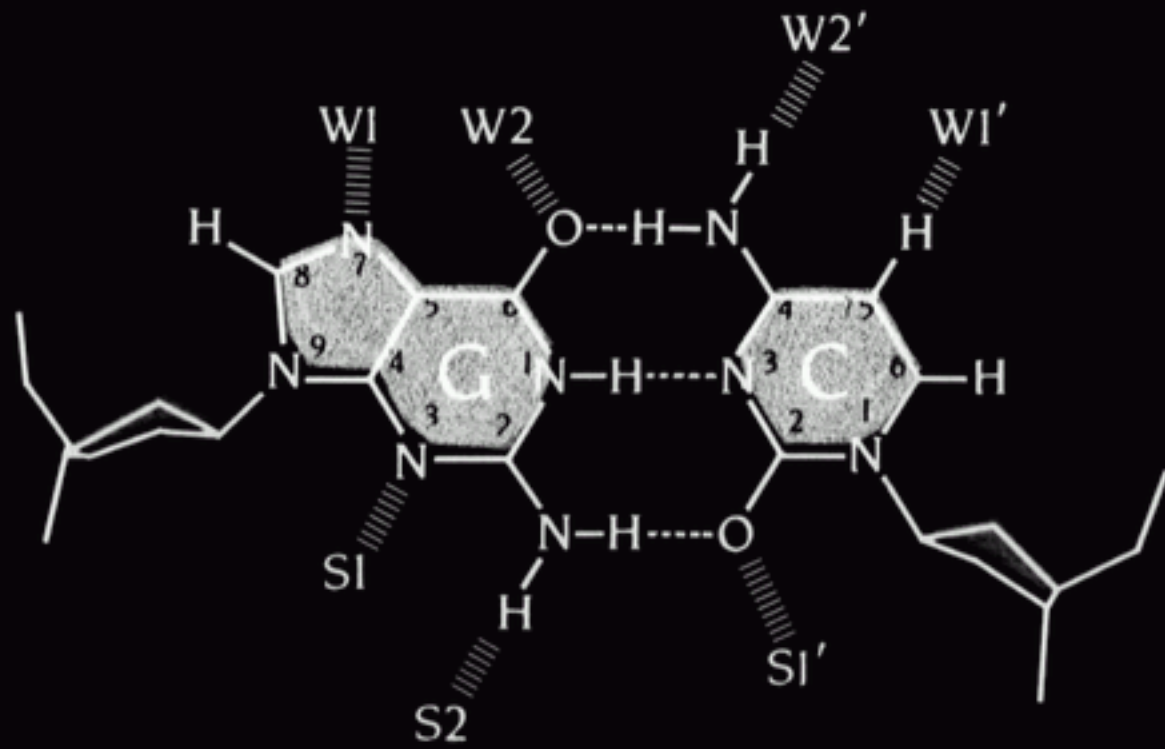
| | |
|-------------|-------|
| X-disp | 0.0 |
| Y-disp | 0.0 |
| Inclination | 1.5 |
| Propeller | -13.3 |
| Rise | 3.38 |
| Twist | 36.0 |

| | |
|-------------------|---------------|
| Tip, Buckle, Open | 0.0, 0.0, 0.0 |
|-------------------|---------------|

| | |
|--------------------|---------------|
| Shift, Slide, Tilt | 0.0, 0.0, 0.0 |
|--------------------|---------------|

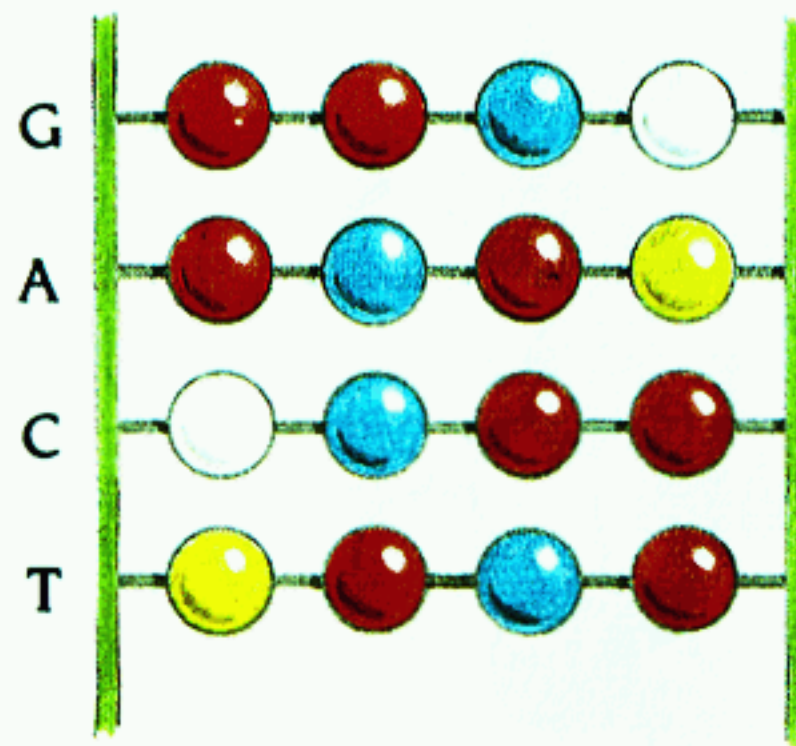
| | |
|------|-----|
| Roll | 0.0 |
|------|-----|

B-DNA, recognition sites



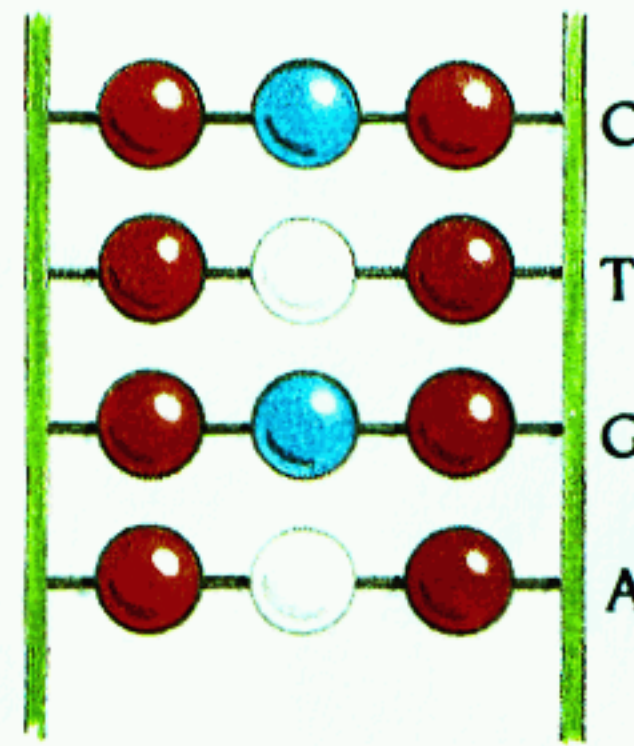
B-DNA, recognition sites

major groove



G - C pair
A - T
C - G
T - A

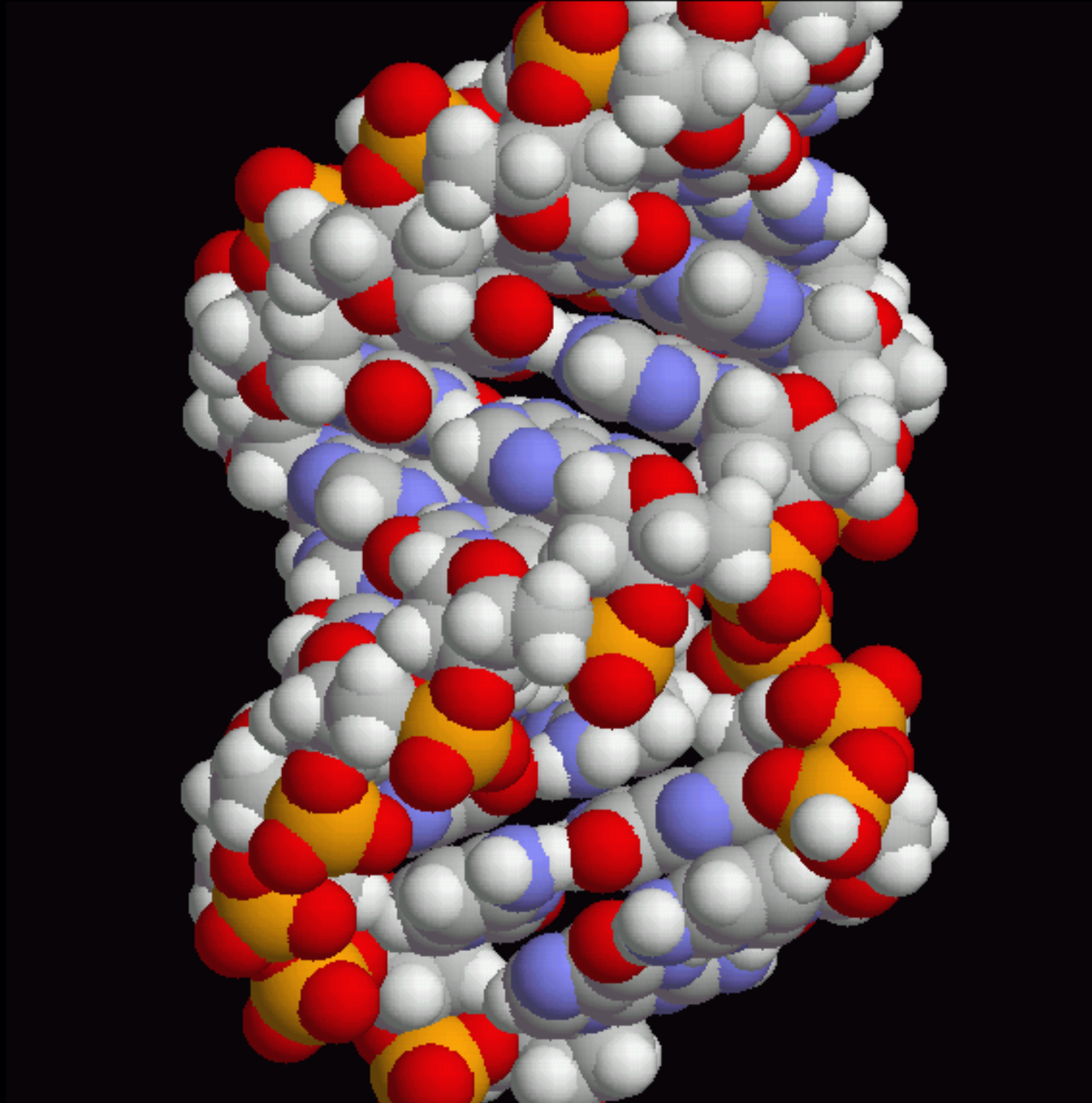
minor groove



KEY

- = H-bond acceptor
- = H-bond donor
- = hydrogen atom
- = methyl group

A-DNA, Watson-Crick bp



A-RNA

C3'-endo

X-disp -5.3

Y-disp 0.0

Inclination 15.8

Propeller 14.5

Rise 2.81

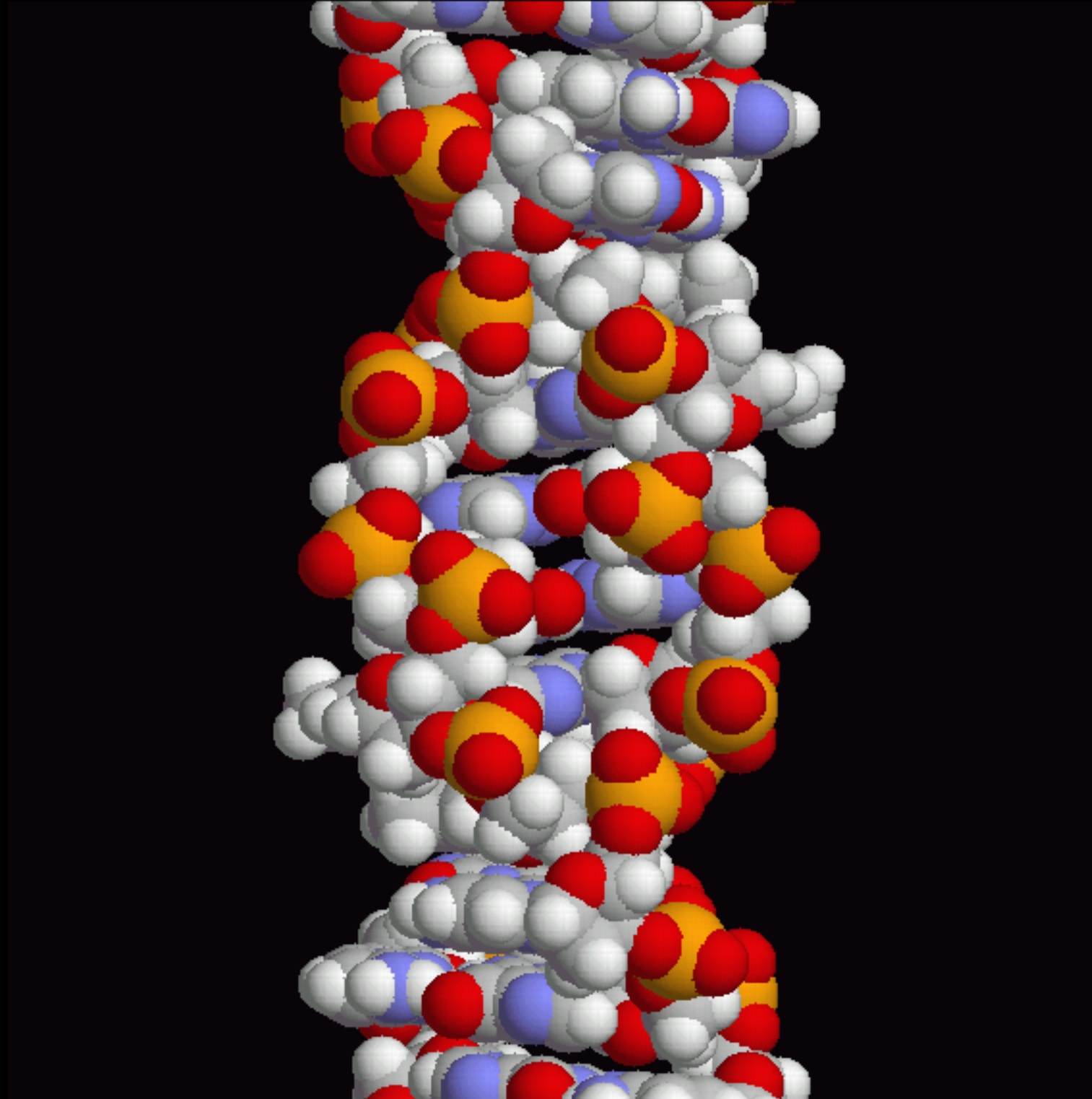
Twist 32.7

Tip, Buckle, Open 0.0, 0.0, -4.2

Shift, Slide, Tilt 0.0, 0.0, 0.0

Roll 0.0

Z-DNA, Watson-Crick bp



Z-DNA

C2'-endo - C3'-endo εναλλάξ

X-disp -2.46

Y-disp 2.32

Inclination 4.2

Propeller -0.8

Rise 3.08

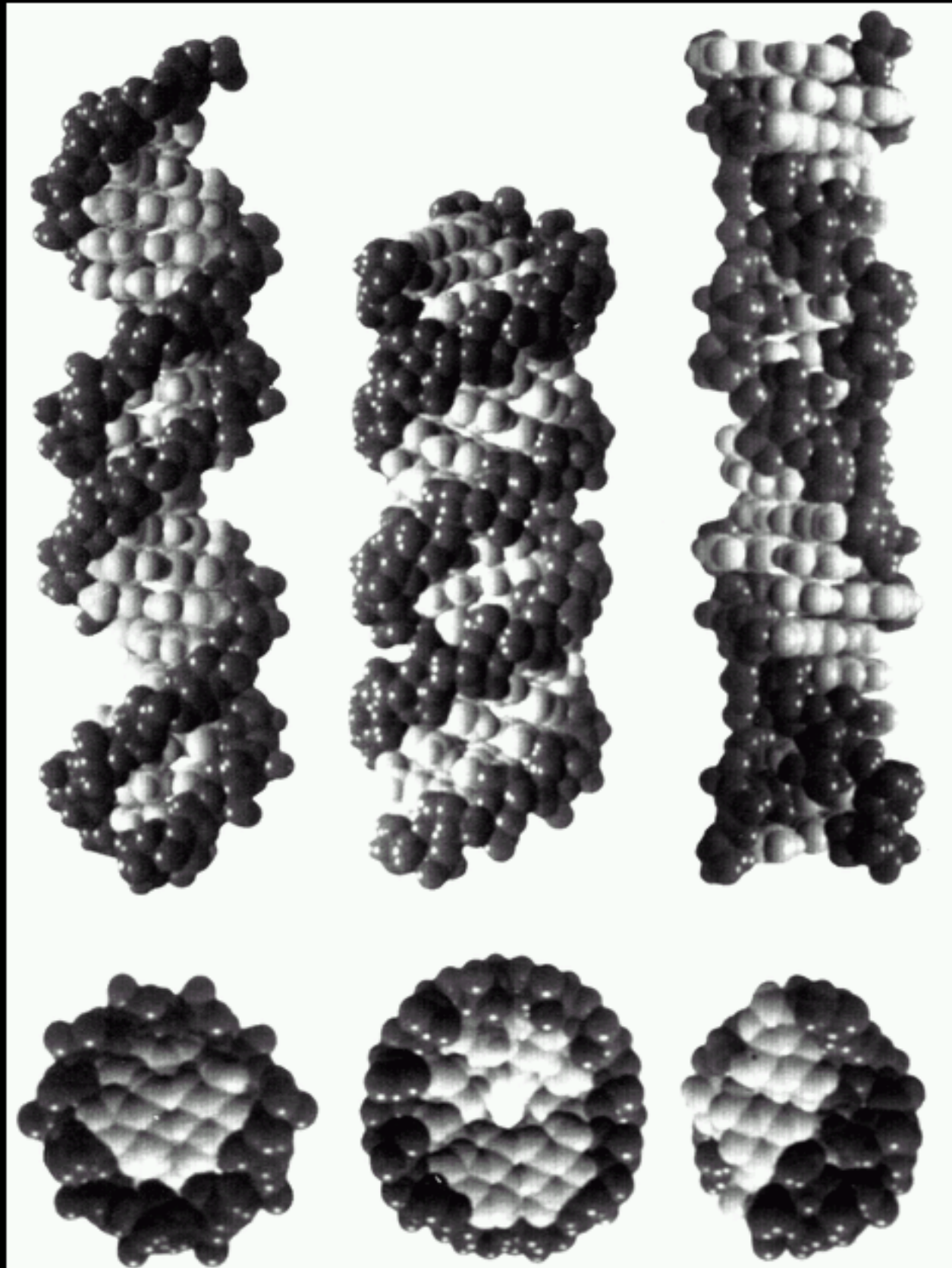
Twist -56.3

Tip, Buckle, Open 178.2, -6.3, 5.6

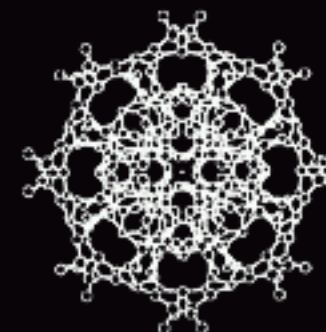
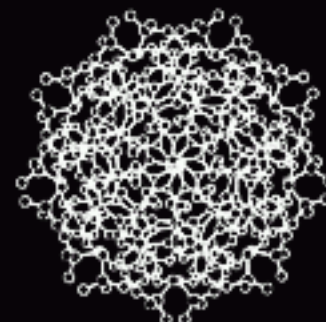
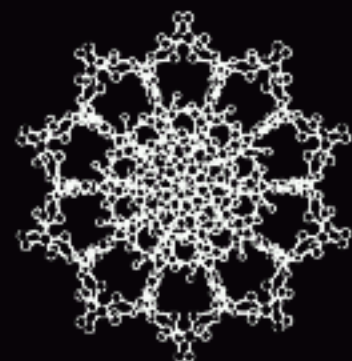
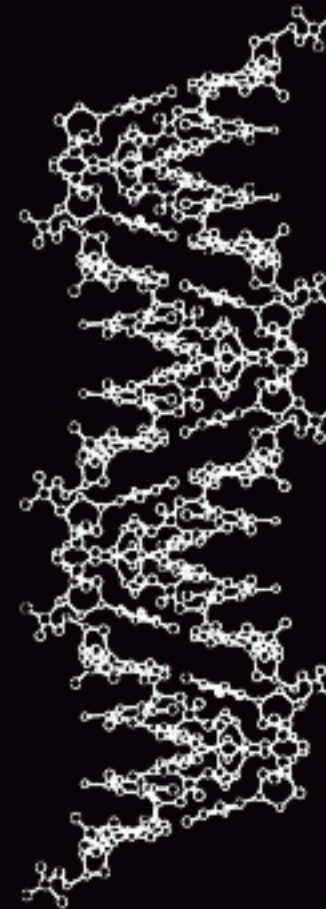
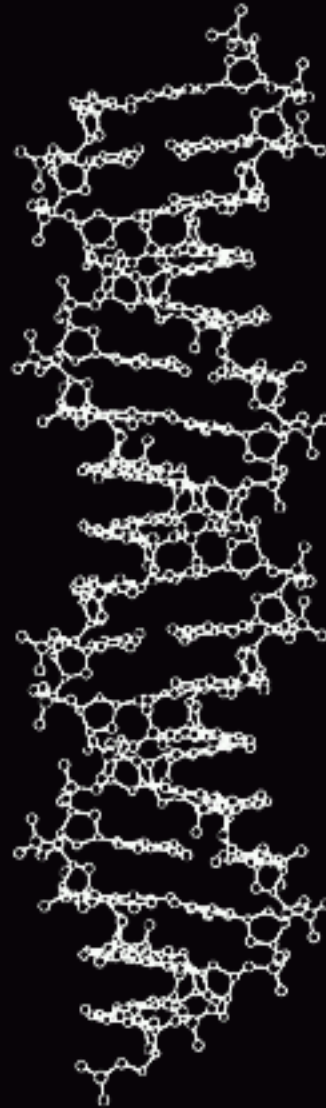
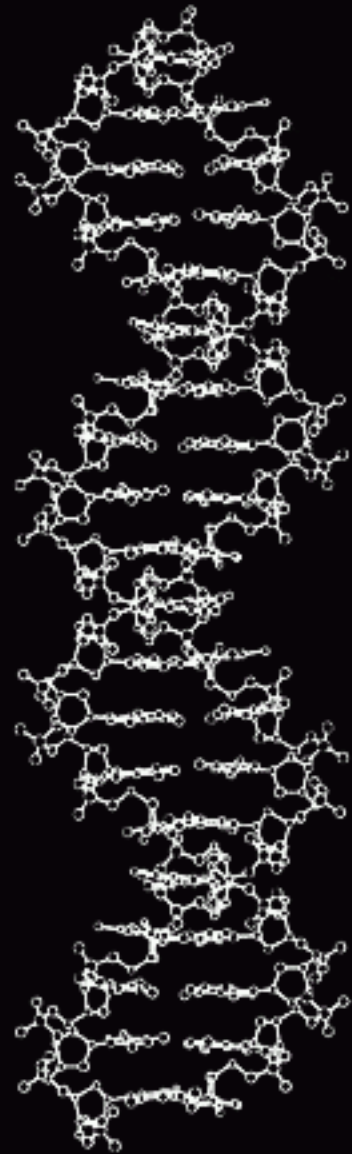
Shift, Slide, Tilt 0.0, -4.63, 0.0

Roll 3.6

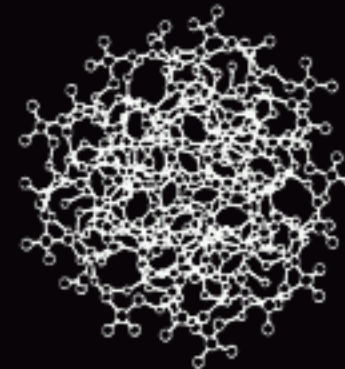
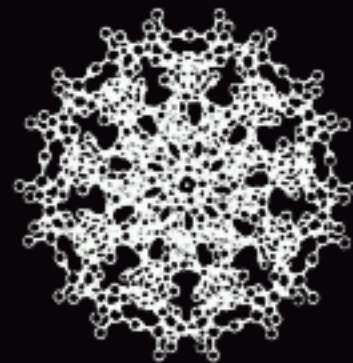
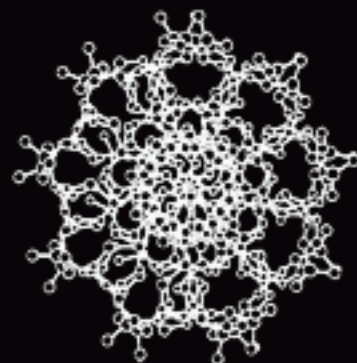
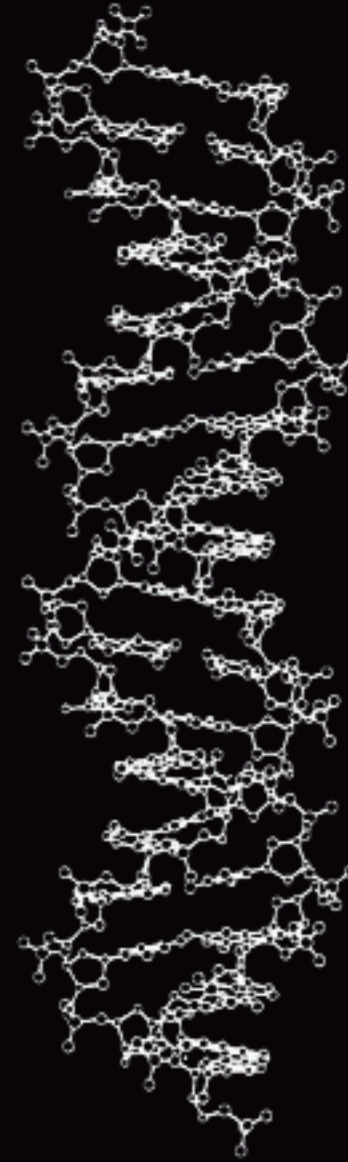
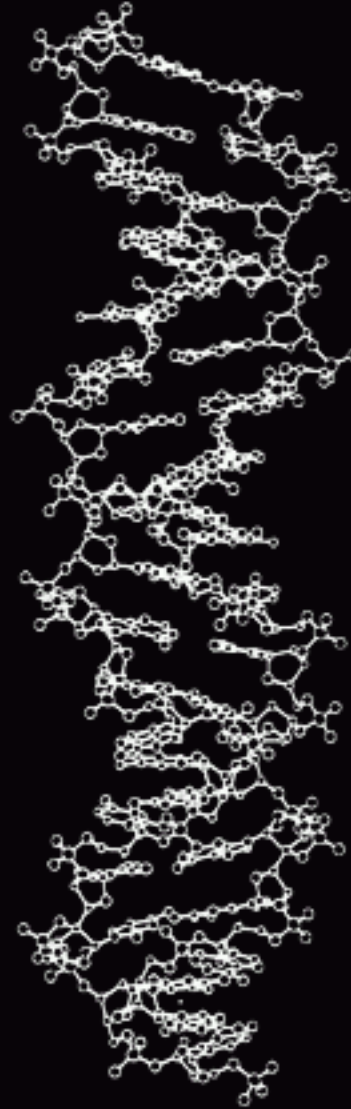
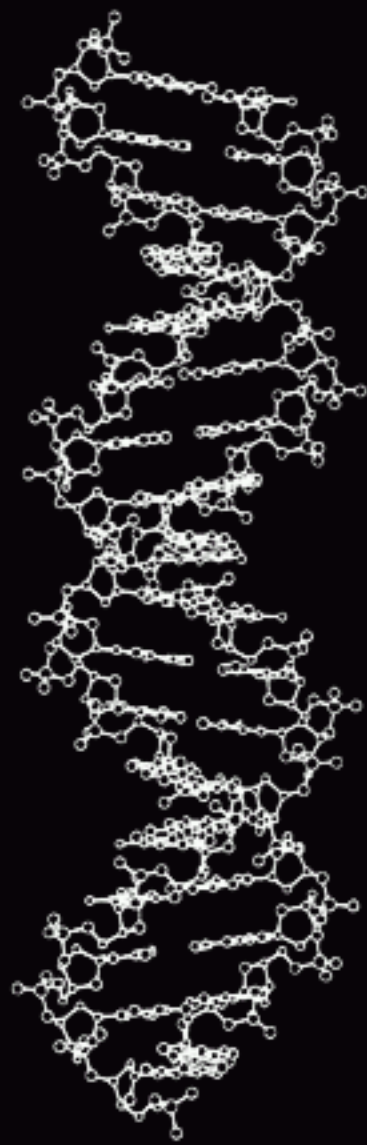
B, A, Z



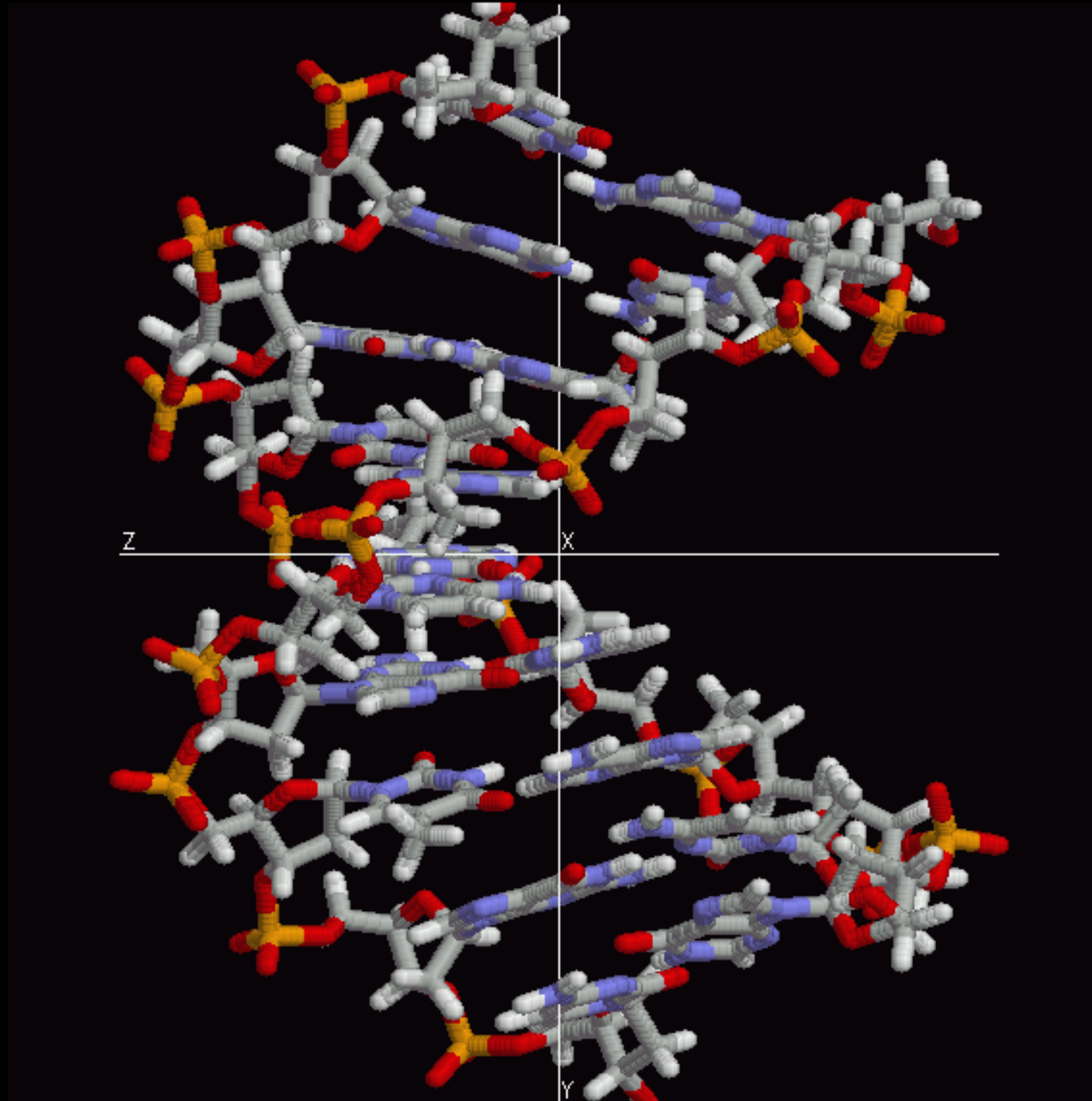
B, C, D



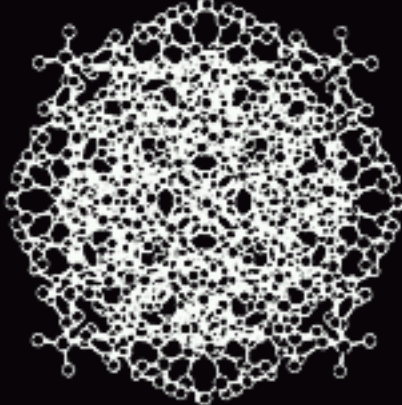
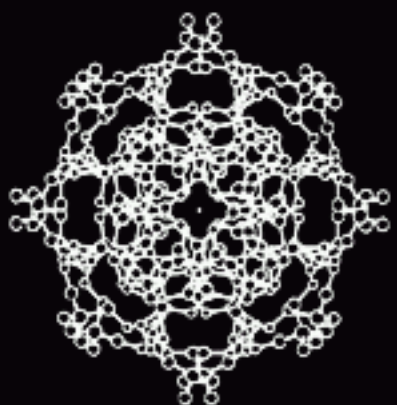
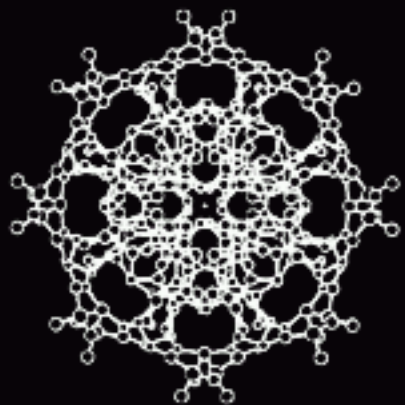
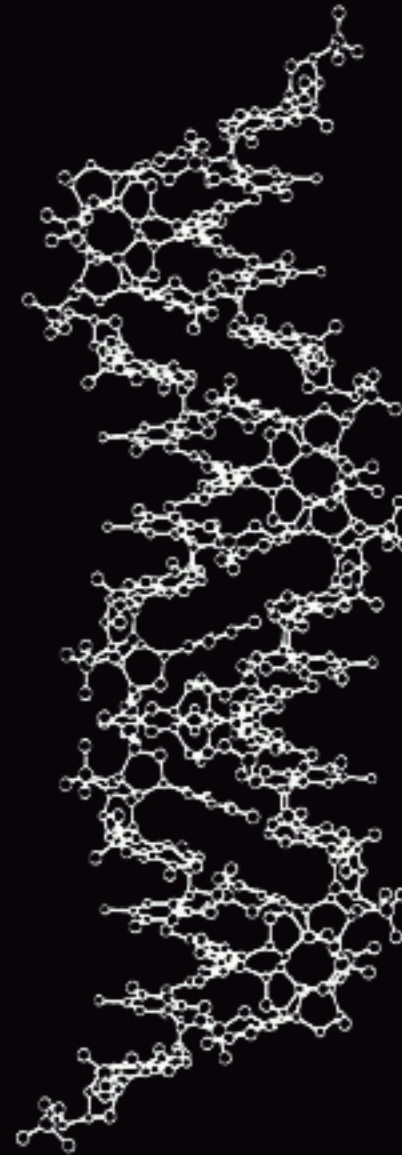
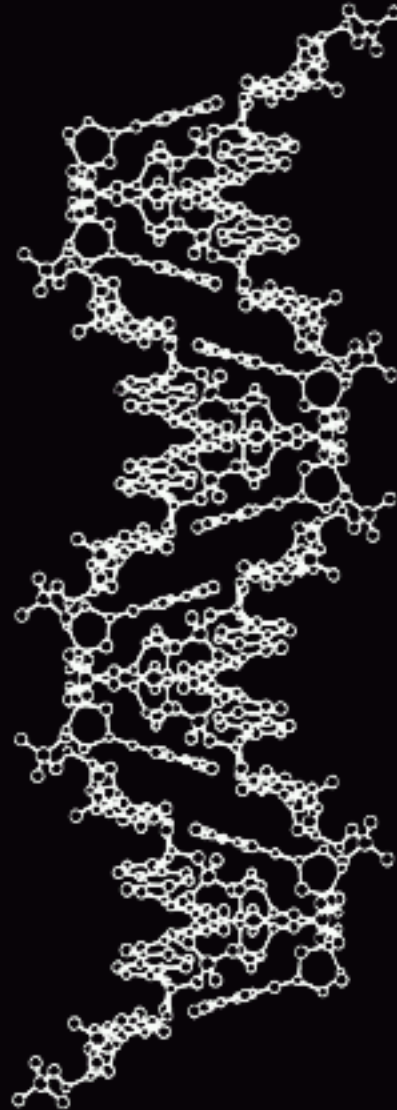
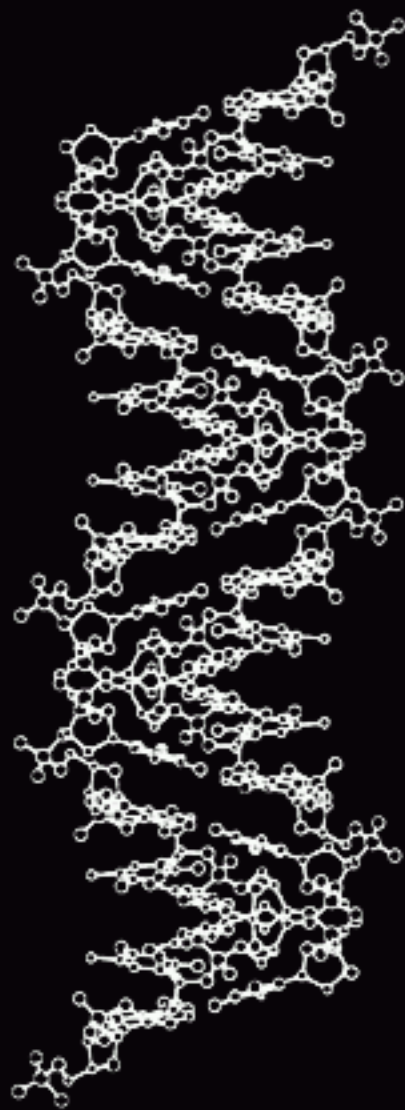
C-DNA



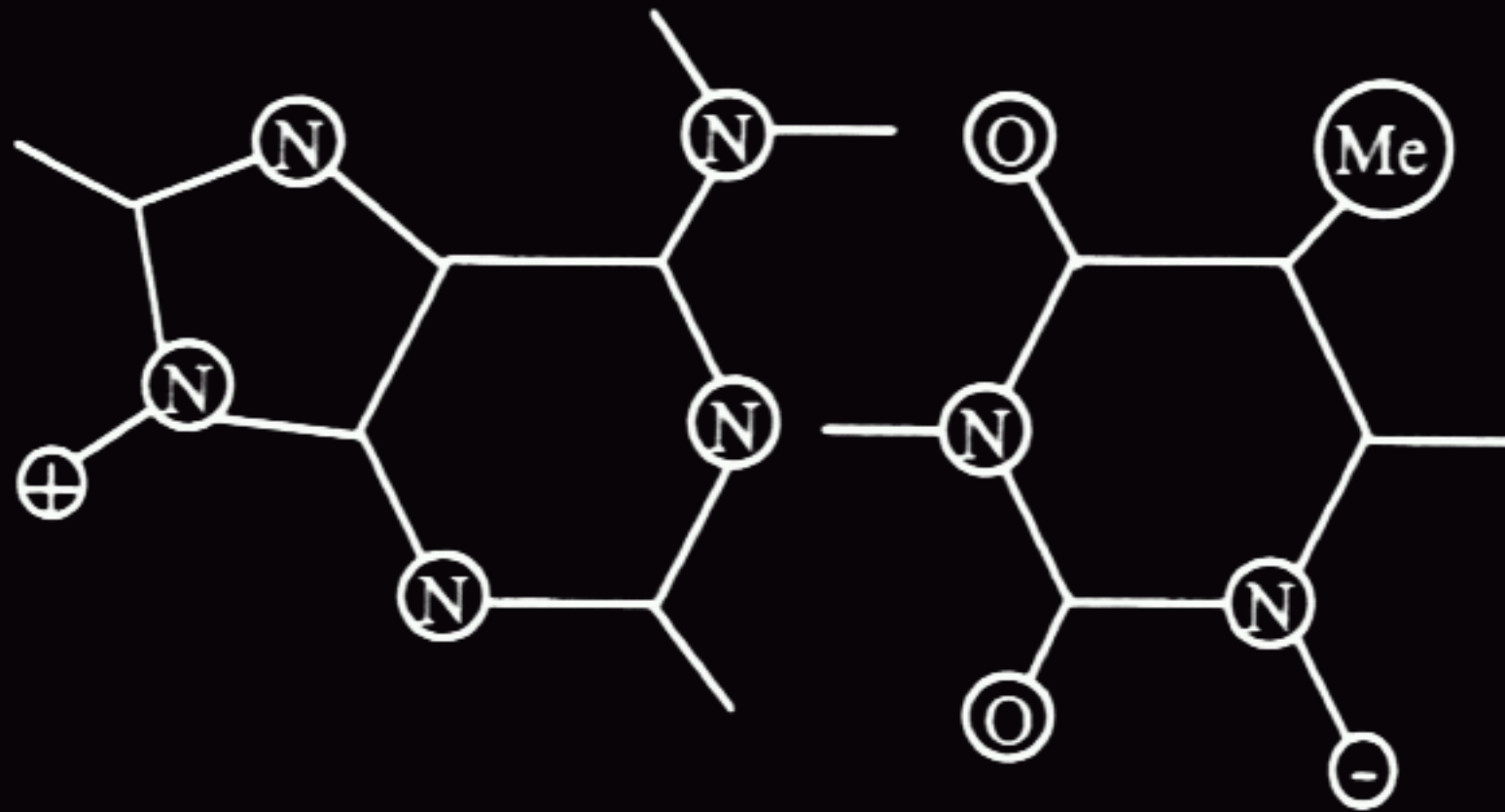
C-DNA, Watson-Crick



D-DNA

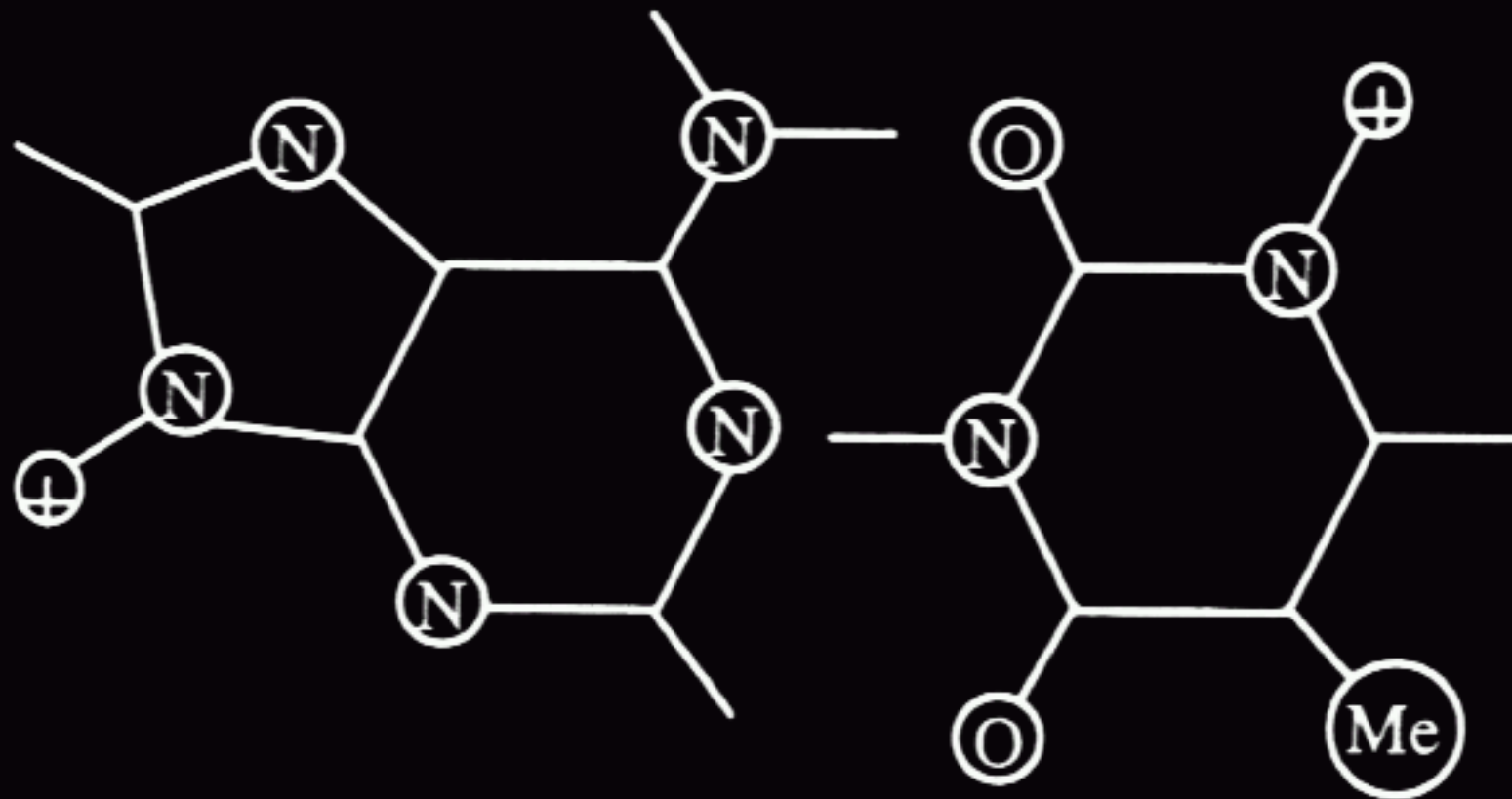


Watson-Crick AT



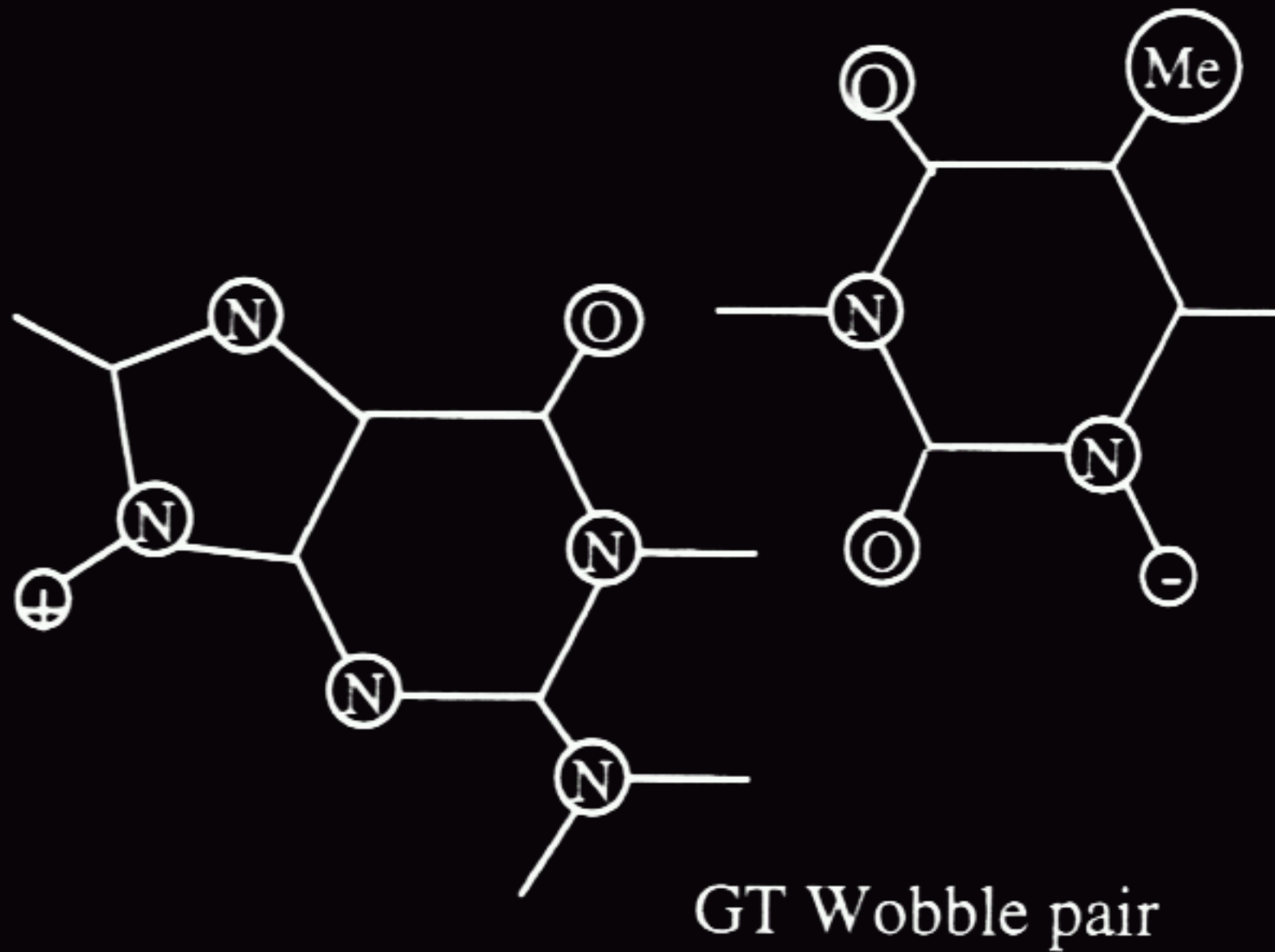
AT Watson-Crick

Reversed Watson-Crick AT

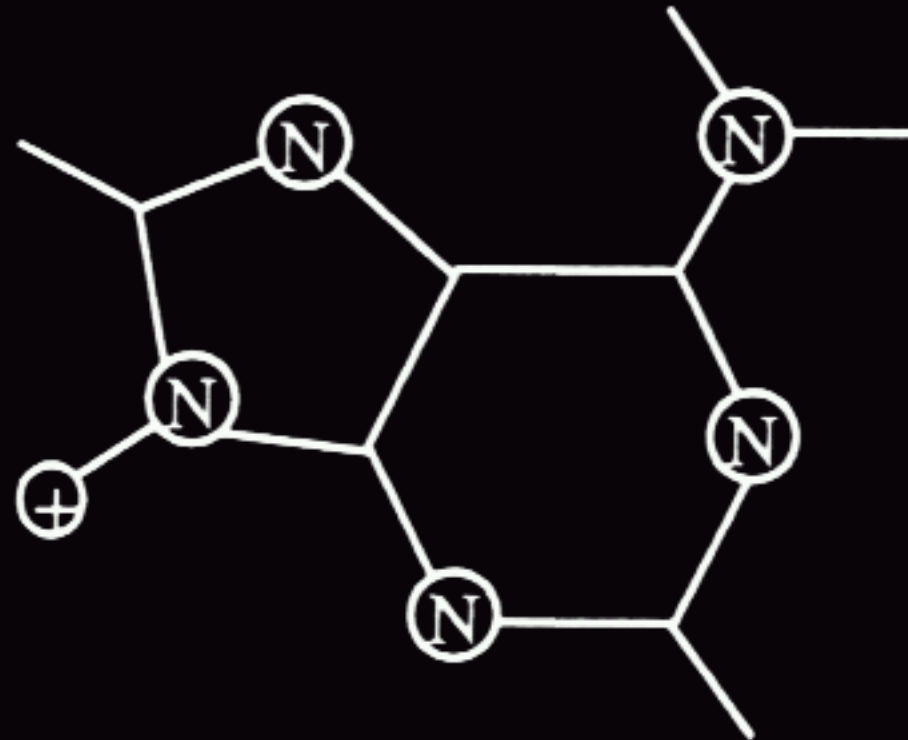
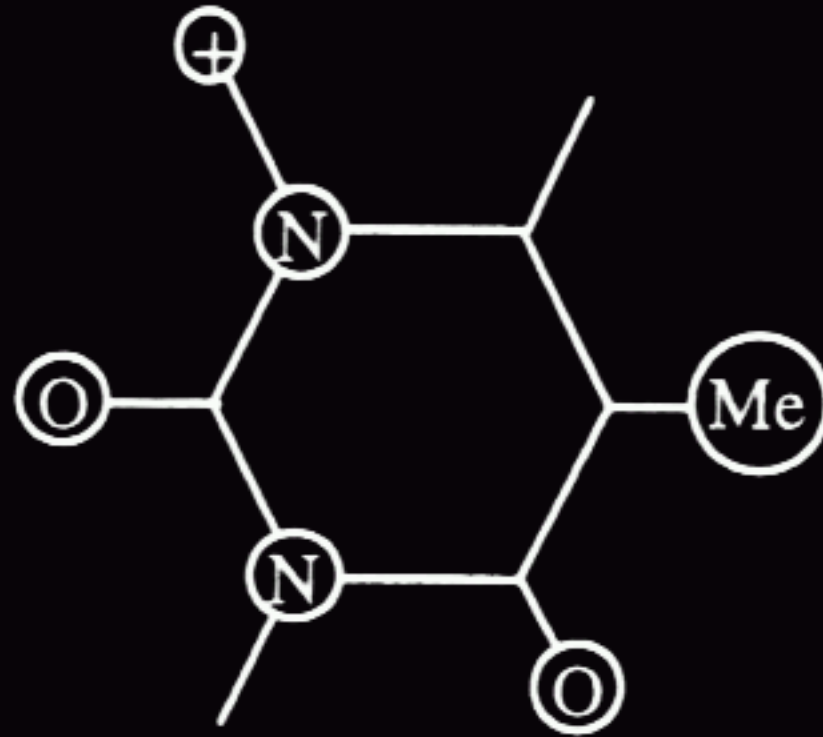


AT Reversed Watson-Crick

GT wobble base-pair

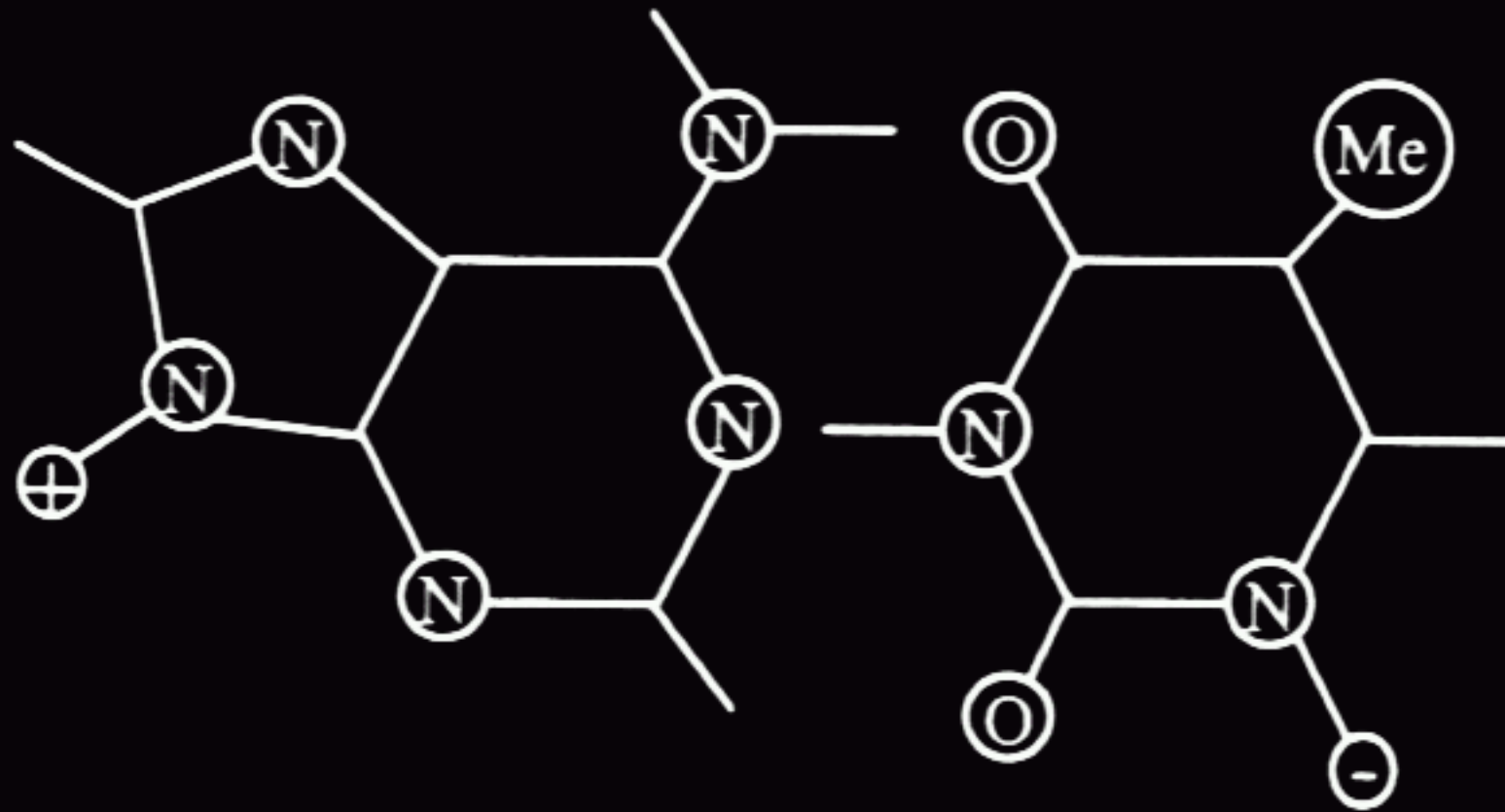


Hoogsteen AT



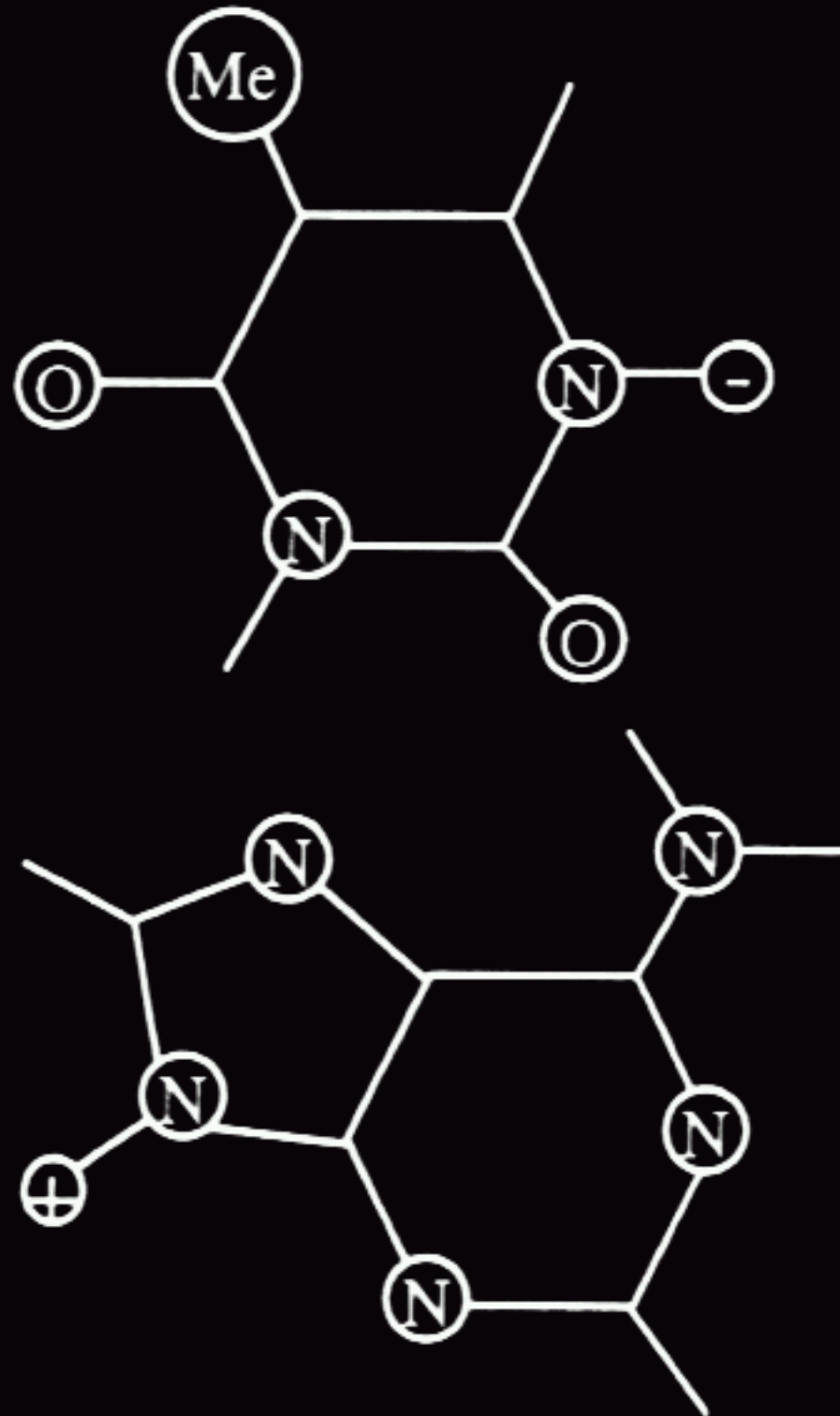
AT Hoogsteen

Watson-Crick AT



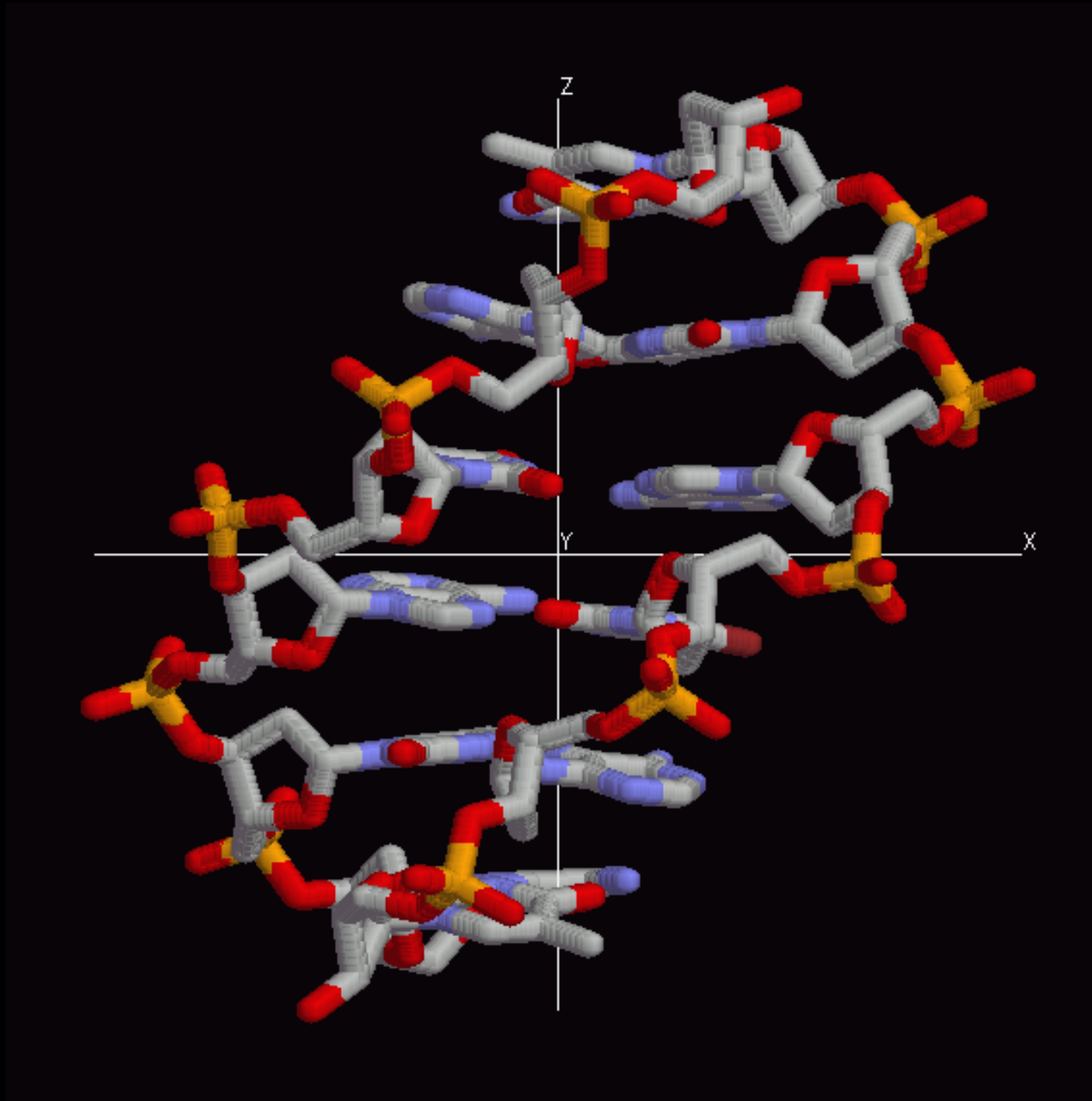
AT Watson-Crick

Reversed Hoogsteen AT



AT Reversed Hoogsteen

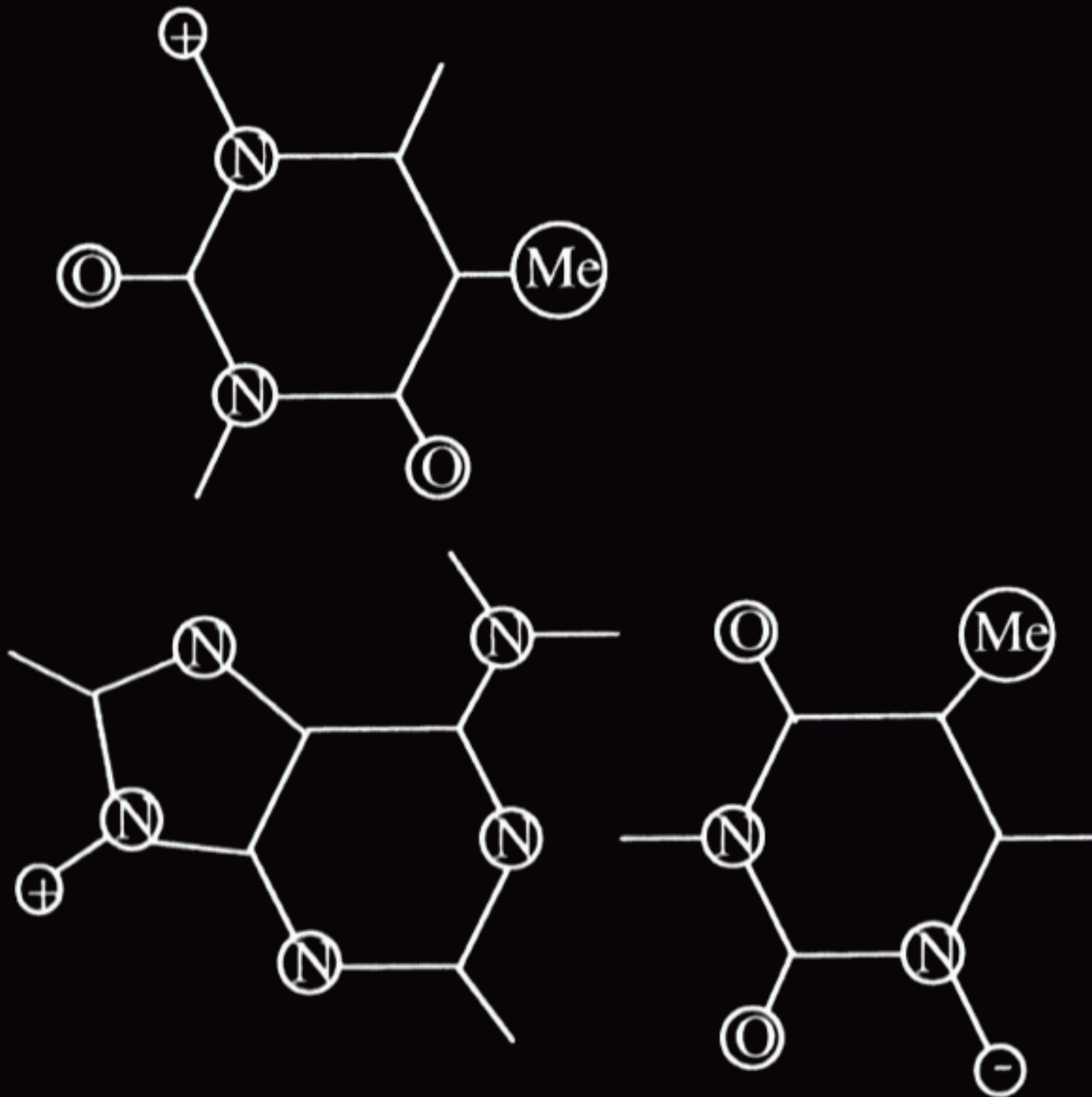
Hoogsteen B-DNA



S47_1

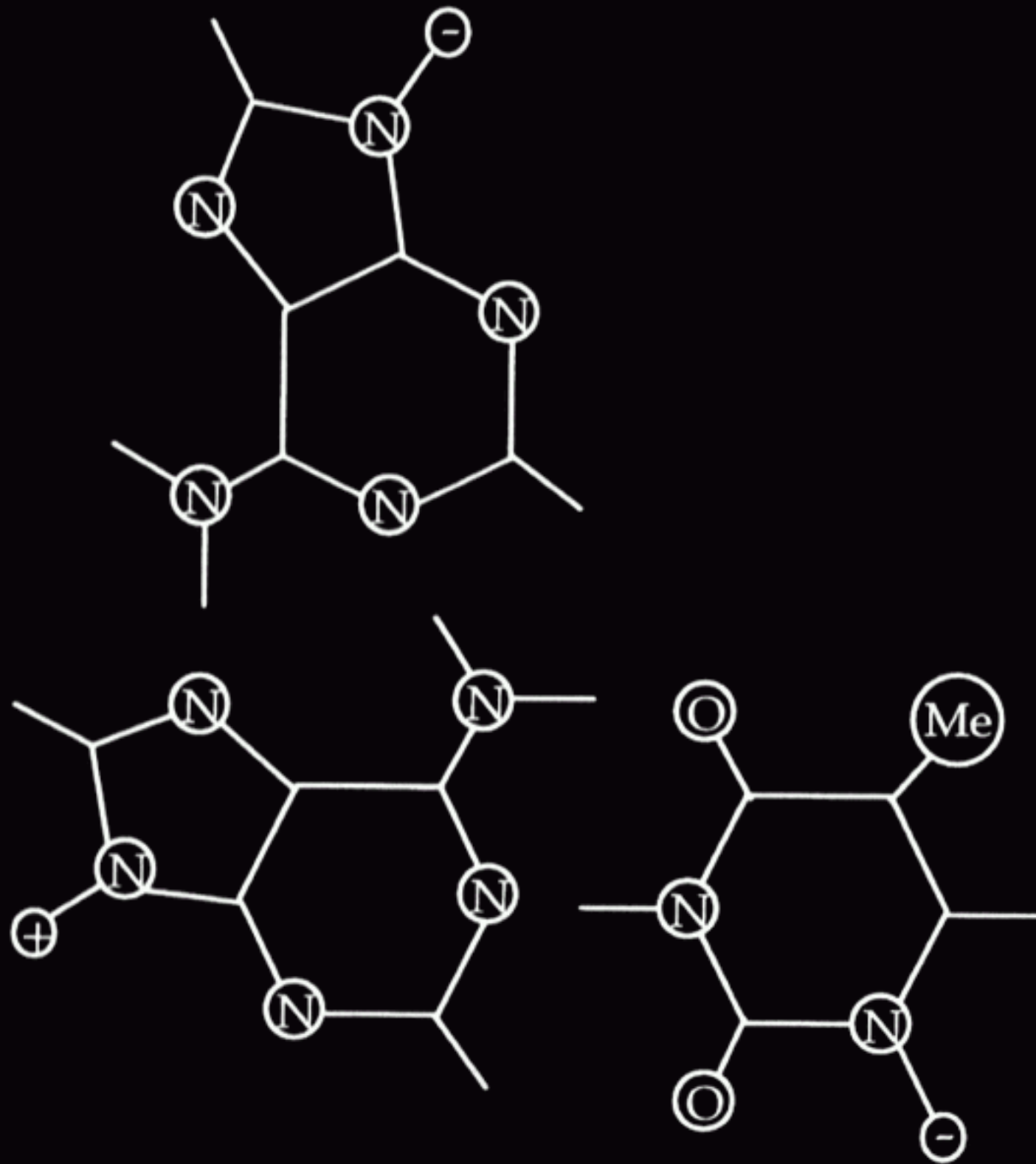
S47_2

Triplexes : T.A x T (Hoogsteen)



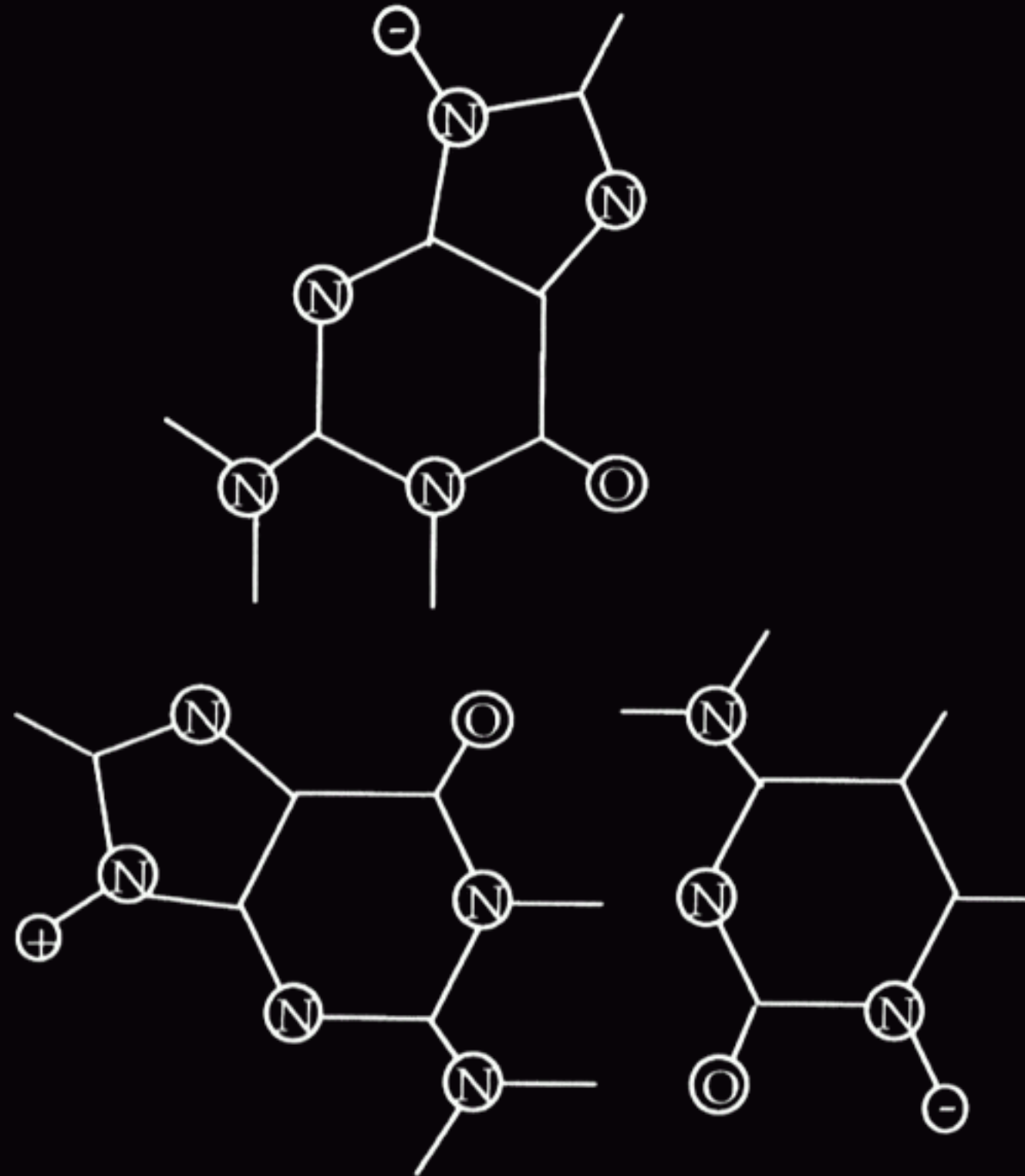
T.AxT Triplet

Triplexes : T.A x A (rev. Hoog.)



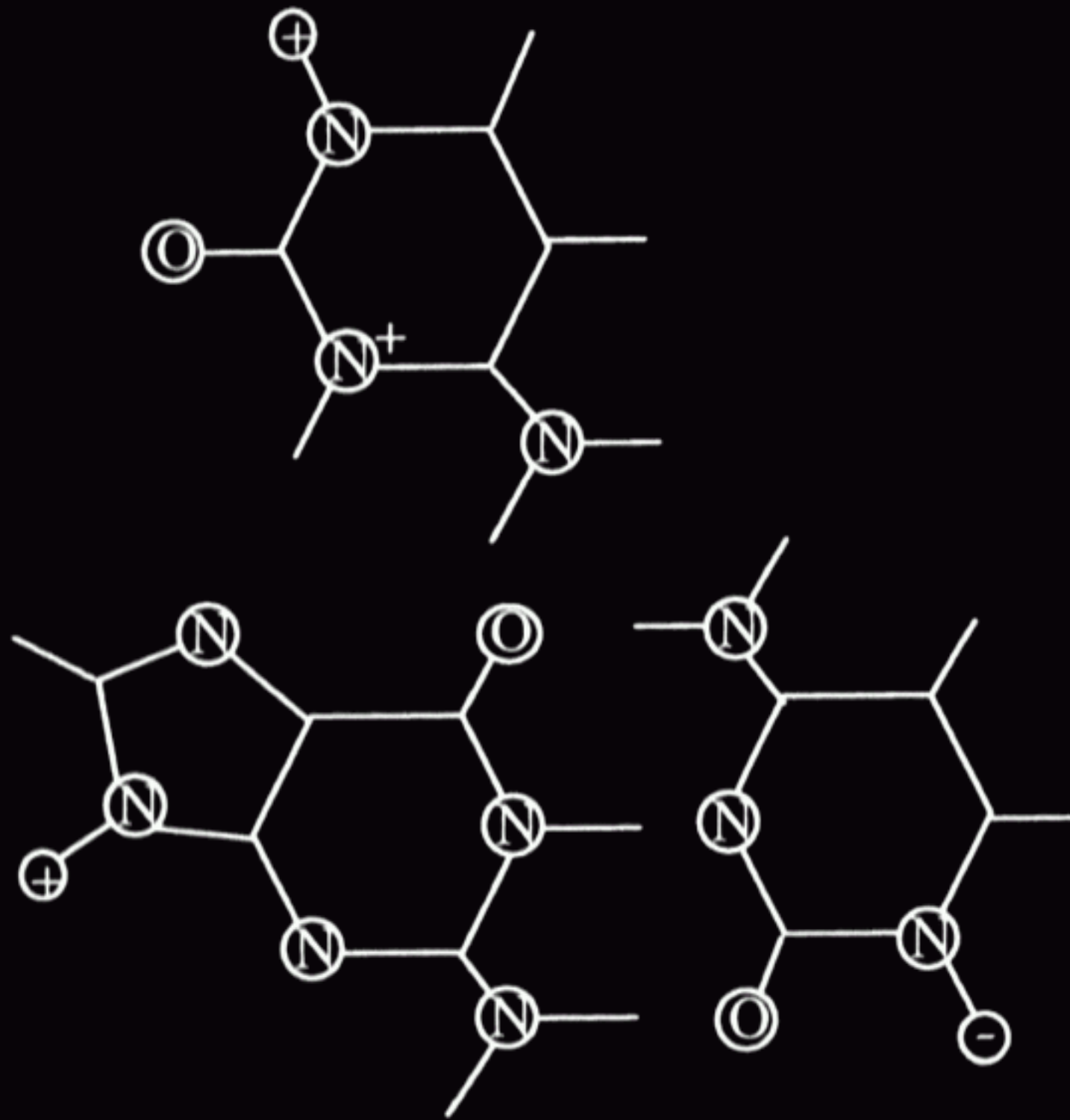
T.AxA Triplet

Triplexes : C.G x G (rev. Hoog.)



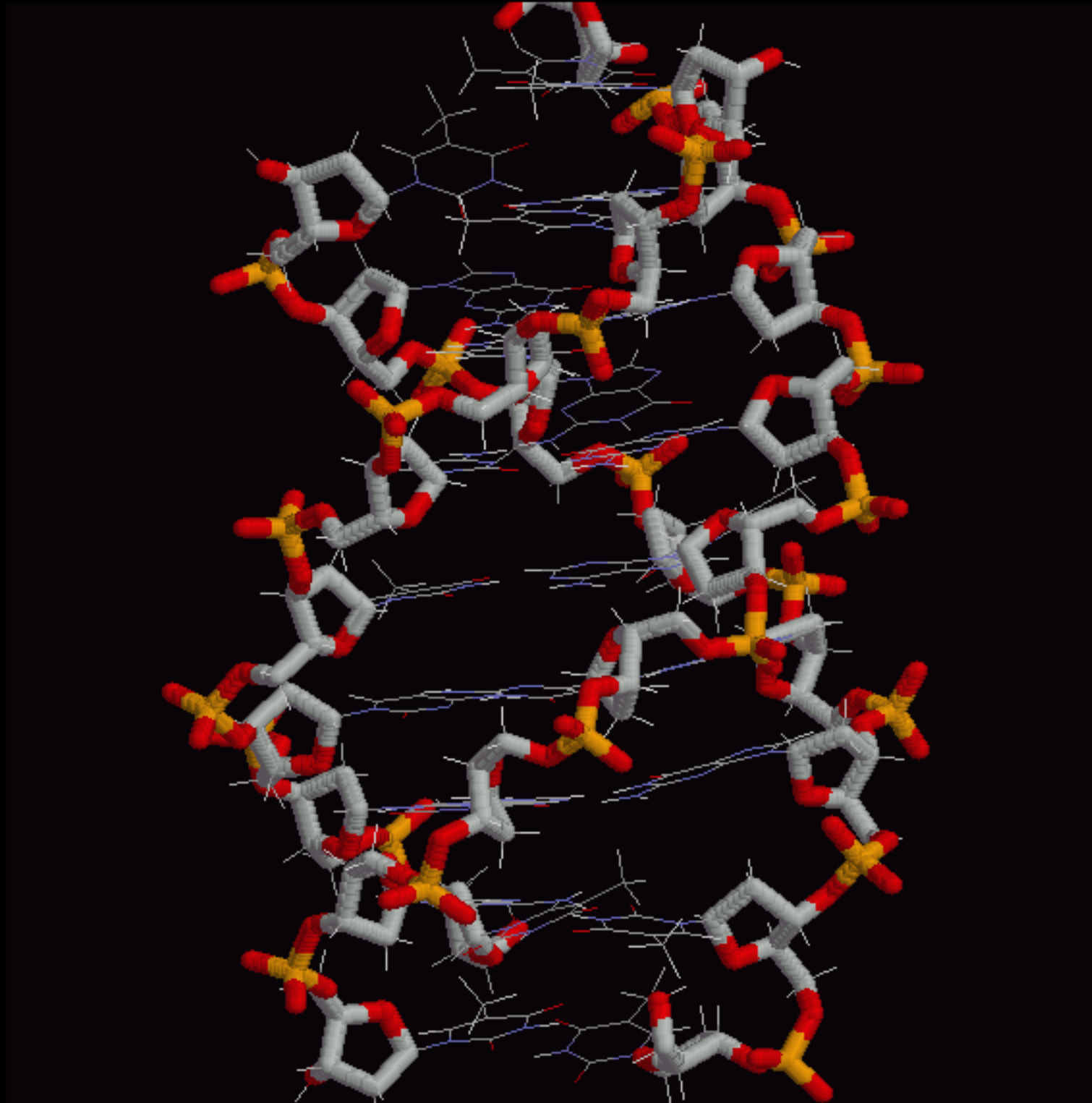
C.GxG Triplet

Triplexes : C.G x C⁺ (Hoogsteen)

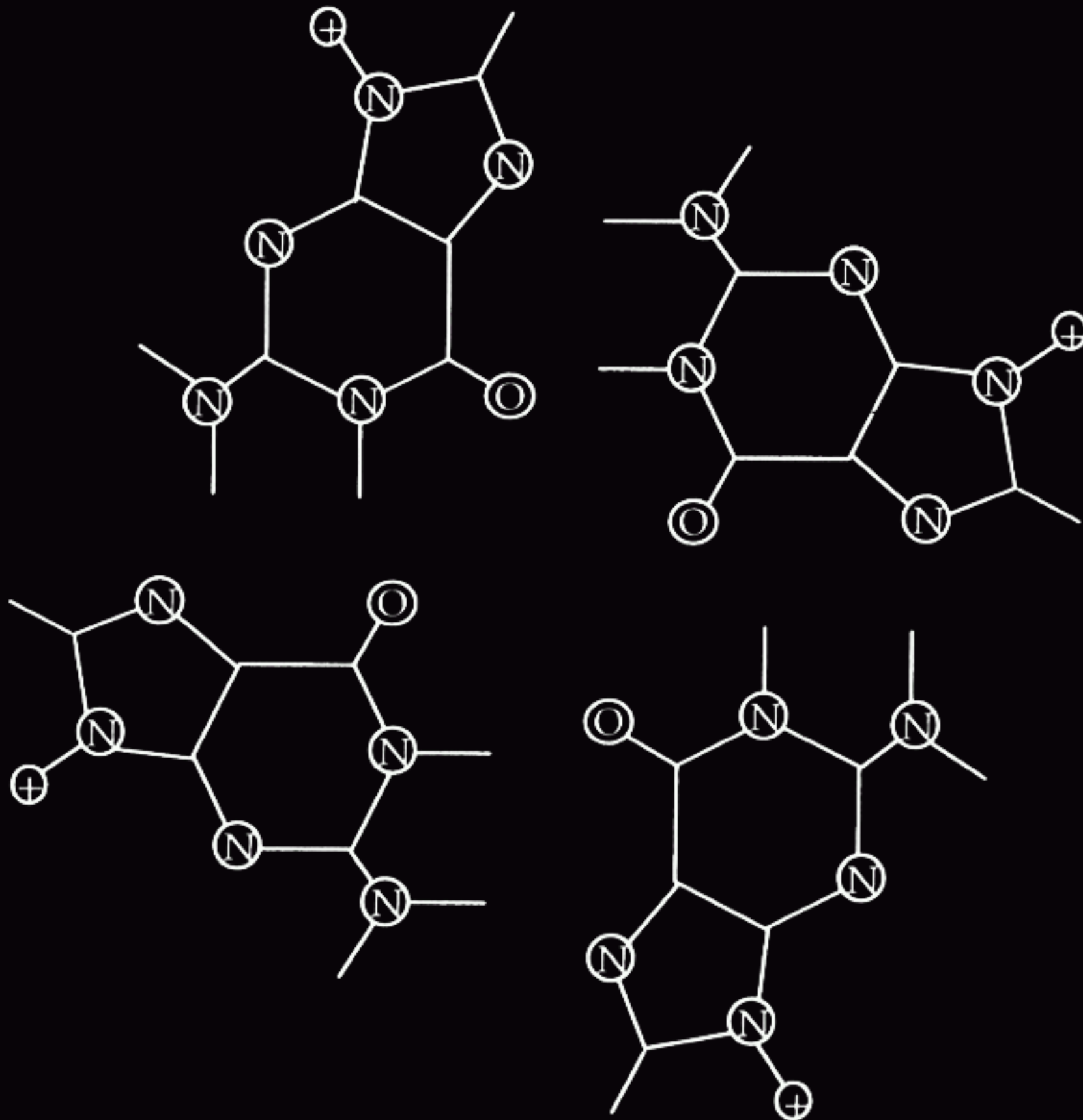


C.GxC⁺ Triplet

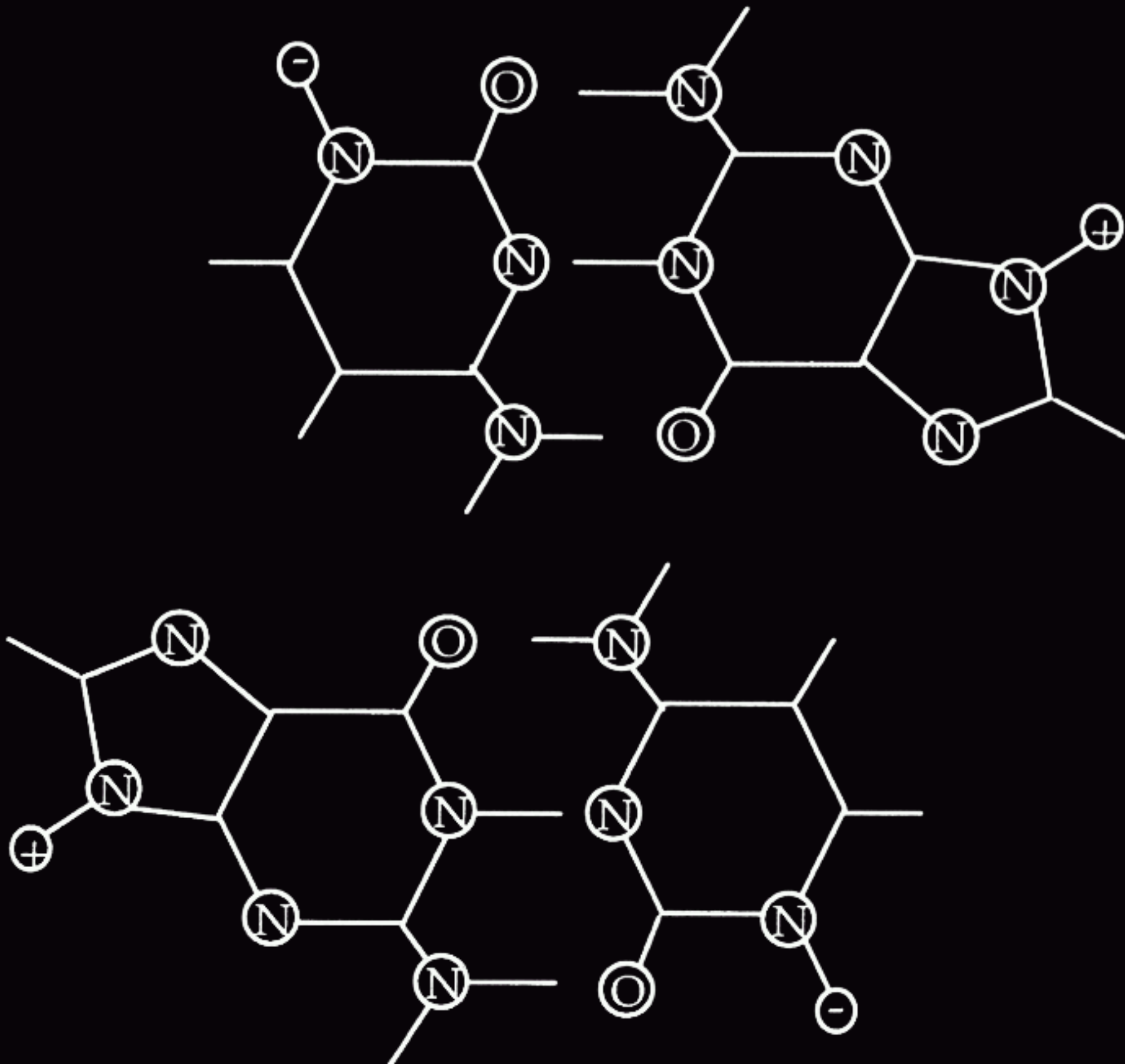
Triplex DNA



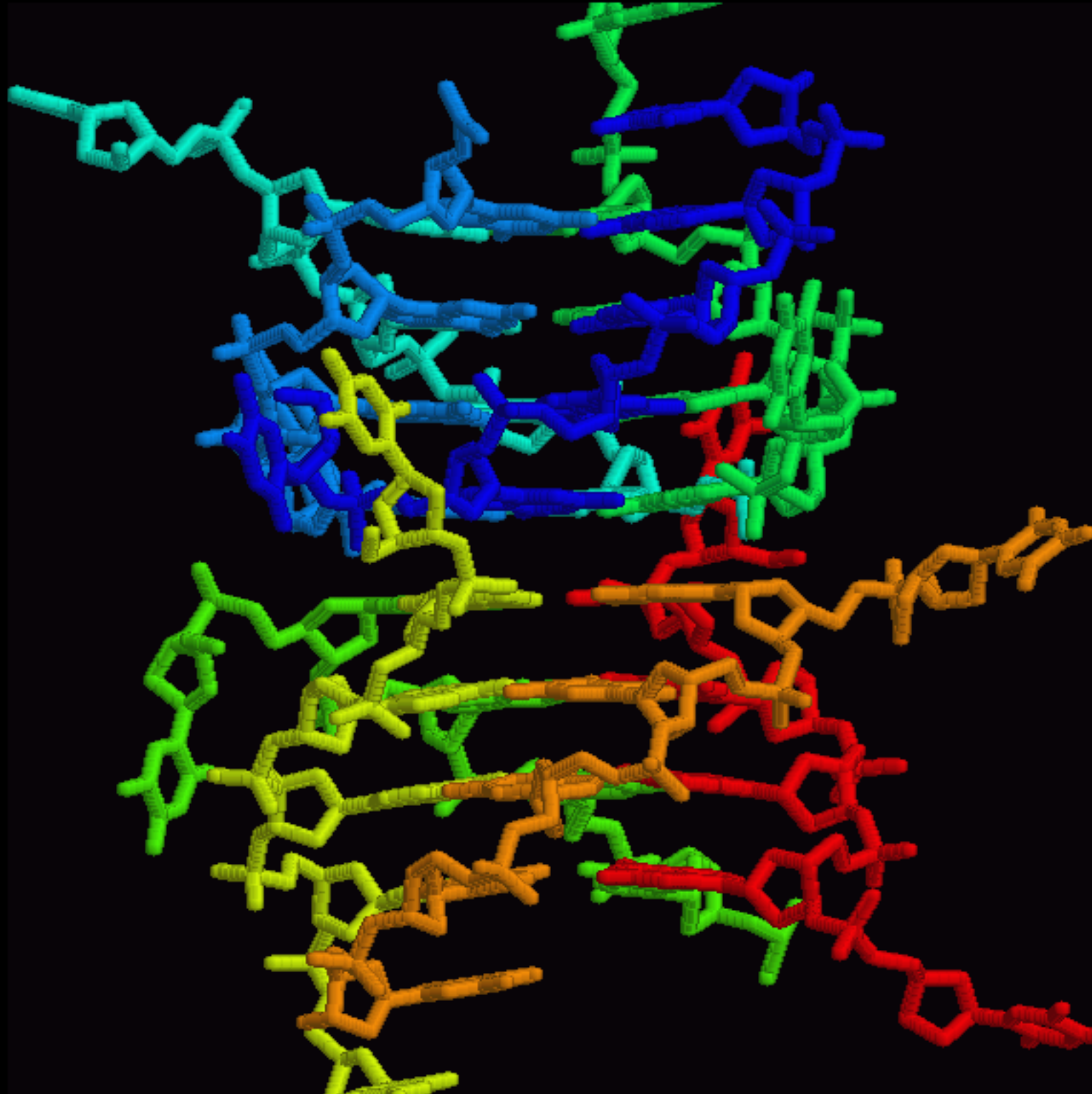
Quadruplexes : G4 (rev. Hoog.)



Quadruplexes : (AT)₂



G4 tetraplex



RNA structures : yeast tRNA(Phe)

