

Do-it-yourself DNA Homework Assignment

This week you will use Molymod™ components to assemble a short section of DNA. This will consist of the backbones with two paired bases (AT and GC). The A and G bases will be on one side of the spiral (attached to two repetitions of the sugar-phosphate spiral backbone units). The T and C bases, in complementary positions, will be attached to the other section of spiral backbone. **The desired structure is shown below in an excerpt from Wikipedia's DNA figure** (note that this figure follows the organic chemistry convention of not showing all hydrogen atoms - you must infer the missing hydrogens' presence from the need to come up with proper number of valence electrons for each atom).

Getting all of this right, with the bases in positions so that two strands fit together properly, is no easy task. So this time you will do the assignment in teams of three.

The parts will again be given to you in a plastic bag. The inventory of what it contains (and some hints as to assembly) are on a separate page below.

The two DNA strands are held together by "hydrogen bonds" which are not bonds in the more conventional sense. When a hydrogen atom forms a normal chemical bond, its one electron is drawn into that bond, to one side. This partially uncovers the proton of hydrogen's nucleus, leaving a net positive charge. In other atoms, such as nitrogen or oxygen, pairs of unbonded electrons may form, giving that region a net negative charge. If a slightly positive hydrogen nucleus *on one molecule* finds itself close to the slightly negative pair of unbonded electrons *on another molecule*, the + and - charges will draw together forming a weaker "hydrogen bond." This combination of charge arrangement and shape (so that the charges come close enough to one another) is what holds the complementary bases of DNA (and hence the two strands) together!

So, to properly represent DNA, this time we really do have to show **all** of the valence electrons: those in conventional sigma bonds, those in secondary pi bonds, and pairs of unbonded electrons.

As a resource in figuring out such details, you are encouraged to consult the "UVA Virtual Lab" webpage on "DNA - close up." Scenes on this webpage download to your PC three-dimensional models of the proper length of sugar-phosphate backbone, of the individual bases (including all the details of the bonds), and the final full two base pair structure:

www.virlab.virginia.edu/VL/DNA_close_up.htm

On this webpage, start by clicking on the second icon to bring up the representation of the individual bases. For each base, click the "Toggle Bonds" button twice to show the full complement of valence electrons and the pi bonds they make. This is the form I want you to assemble (one more click on that button shows the electrons after they "delocalize" spreading into the rings)

In assembling your model, follow these rules:

- Use the standard atom color code of:

Carbon = black Hydrogen = white Oxygen = red

Nitrogen = blue Phosphorus = purple

- The atoms in your kit have holes for all of the valence electrons (except for oxygen – see note 2 below) and **every hole should be filled!!**

- For a simple single sigma bond between atoms, use a single (short fat) bond

- For a double sigma + pi bond, loop two (long skinny) bonds between the atoms. This is not quite accurate, and not quite the way that it is depicted on the webpage (where the full sigma+pi structure is shown), but it works well with these Molymod atoms.

- For an unbonded PAIR of electrons (as will occur on many of the base nitrogens and on one of each phosphate groups' oxygens) place a purple half bond in one hole of an atom (this corresponds to the fat electron pairs shown on the webpage)

There are two anomalies in the kits:

1) The phosphorus atoms in the phosphate backbone units actually end up having five bonds (three single bonds to O's, one double bond to an O). But the Molymod P atoms don't come with five bonding holes – so I have personally drilled out new holes (and filled one of the old) to allow for the double bond.

2) The oxygens should have holes to accommodate all six of their valence electrons. But as only two of the electrons bond (the other four form non-bonding pairs) Molymod oxygen atoms come with only two holes for the bonding electrons (i.e. the two non-bonding pairs are omitted).

If you have constructed your model correctly, almost all atoms should be neutrally charged:

Then for each atom you should find the proper number of valence electrons by attributing to that atom one electron for each bond (i.e. each atom “owns” one of the pair of electrons in the bond to a neighbor), and two electrons for an unbonded pair (which are totally “owned” by that atom). If you get it right (yielding net zero charge on that atom), you will have:

H = 1 valence electron

C = 4 valence electrons

N = 5 valence electrons

P = 5 valence electrons

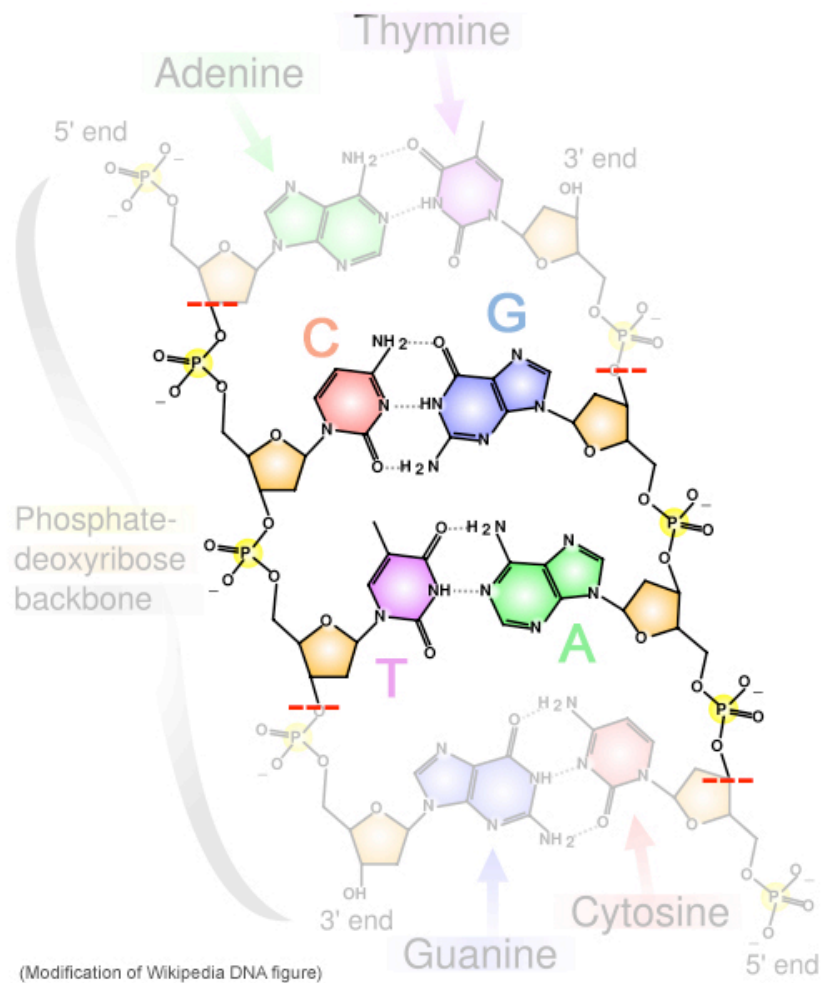
O = 6 valence electrons (except here Molymod atoms hide the two non-bonding pairs, per note 2 above)

All but four atoms in your model should indeed end up neutral! The exception is that on each phosphate group there will be one oxygen atom with a net negative charge of one. This is real and this charge on the DNA backbones tries to push the two strands apart. The delicate balance between backbone repulsion and base hydrogen-bonding, makes DNA strands easy to separate – which is rather important if they are to do their job!

Additional Requirements:

These kits are even more costly than last week's nanocarbon kits, so when you submit the assignment we will again count or weigh what you return to make sure nothing has been lost (expecting you to replace any such losses out of your own pocket).

Submit the assignment with the Honor Code pledged sheet below.



DNA kit contents:

Two sections of ribose-phosphate backbone (each with two repetitions of the ribose + phosphate):

	20	4-bond (sp ³) black carbon atoms
	4	5-bond purple phosphorus atoms (my special modification)
	20	2-bond red oxygen atoms
	28	1-bond white hydrogen atoms
	74	Short grey bonds
	8	Long grey bonds (for the doubly bonded oxygen in each phosphate group)
	4	Purple half bonds (unbonded electron pairs on one oxygen in phosphate group)
Adenine:	5	4-bond black carbon atoms
	5	4-bond blue nitrogen atom (2 in each rings + side group)
	0	2-bond red oxygen atoms
	4	1-bond white hydrogen atoms
	12	Short grey bonds
	8	Long grey bonds (four double bonds in rings)
	5	Purple half bonds (unbonded electron pair on nitrogens)
Cytosine:	4	4-bond black carbon atoms
	3	4-bond blue nitrogen atom (2 in ring plus die group)
	1	2-bond red oxygen atoms
	4	1-bond white hydrogen atoms
	10	Short grey bonds
	6	Long grey bonds (2 double bonds in ring + double bond to oxygen)
	3	Purple half bonds (unbonded electron pair on nitrogens)
Guanine:	5	4-bond black carbon atoms
	5	4-bond blue nitrogen atom (2 in each ring + side group)
	1	2-bond red oxygen atoms
	4	1-bond white hydrogen atoms
	13	Short grey bonds
	8	Long grey bonds (three double bonds in rings)
	5	Purple half bonds (unbonded electron pair on nitrogens)
Thymine:	5	4-bond black carbon atoms
	2	4-bond blue nitrogen atoms (two in ring)
	2	2-bond red oxygen atoms
	5	1-bond white hydrogen atoms
	12	Short grey bonds
	6	Long grey bonds (1 double bonds in ring + 2 double bonds to oxygen)
	2	Purple half bonds (unbonded electron pair on nitrogens)

Yielding totals for DNA kit

4-bond (sp ³) black carbon atom:	39
4→5 -bond purple phosphorus atoms:	4
4-bond blue nitrogen atoms:	15
2-bond red oxygen atoms:	24
1-bond white hydrogen atoms:	45
Short grey bonds:	121
Long grey bonds:	36
Purple half bonds:	19

Do-it-yourself DNA Homework Assignment

Did you assemble this kit in a UVA public place (1 bonus point)? _____

Homework Team Member 1)

Printed Name: _____

Check one:

_____ We all contributed significantly to the construction of this model

_____ I did all or almost all the work

_____ I did little or no work

Signature (backed by the Honor Code) _____

Homework Team Member 2)

Printed Name: _____

Check one:

_____ We all contributed significantly to the construction of this model

_____ I did all or almost all the work

_____ I did little or no work

Signature (backed by the Honor Code) _____

Homework Team Member 3)

Printed Name: _____

Check one:

_____ We all contributed significantly to the construction of this model

_____ I did all or almost all the work

_____ I did little or no work

Signature (backed by the Honor Code) _____