Thinking in Blue

Introduction

Some questions ask for you to simply recall facts (what is 2 x 3?), while other questions ask you to apply concepts and processes to new situations (what is 145.8 x -32.5?). CHEM 210 questions all fall into the second category, particularly at the exams, where we use open response (i.e., not multiple choice).

Answering the second type of question takes place in 3 stages:
   (1) diagnose or identify, from the text and drawings of the question, what is the topic or idea
   (2) recall, from your study, the concepts associated with that topic
   (3) apply, based on practice, the concepts to the particulars of the question

This process can be quite new for students, as many introductory science classes often rely on the recollection of facts and information (again… multiple choice testing encourages this).

Bottom line: do not seek out only the answers to practice questions as though those questions or specific facts will re-appear again on new exams as things to recall. They will not. Ever. We use the second type of question on our exams. And when you over-focus on the answers to questions, you can miss the clues and thought processes that go into analyzing the presented information and deciding how to actually answer it!

In Thinking in Blue, some representative questions (many from the text) are taken through the 3-step process in detail: (1) the text and drawings are analyzed for the concepts that need to be gleaned from the page, then (2) a summary of the conceptual information that needs to have been learned, followed by (3) the application of those concepts to the specific question.

Although all the steps are critical, the second step (learning the concepts) is important because these are your critical tools to truly learn and recall. There is absolutely no clue whatsoever about the facts and process that will appear on the page. In other words, you might be able to recognize (what is 145.8 x -32.5?) as a multiplication problem, but if you do not know how to multiply, there is nothing at all in the question that can help you out… and all the memorized examples in the world are useless unless one of them happens to be “145.8 x -32.5”!

A few principles, then:

(a) information in the question should elicit the identification of which concept(s) are needed
(b) identified concept(s) set up expectations for what you should be carrying in from your learning
(c) the concept you carry in needs to be applied to the information of the question

AND

(A) an answer needs to make internally consistent sense with respect to all the information
(B) as you are learning, any source of only an answer, regardless of its source (answer keys, peers, GSIs, professors) will miss the problem-solving process – an “answer” is the destination

Thinking in Blue is intended to illustrate explicitly the value of the problem-solving process – what a person needs to be thinking about to get to an answer, which is the expertise you develop from learning anything.

What is usually provided as a direct answer to the question is presented in red.

What you need to be thinking about is presented in blue.
Trichalcogenasumanene orthoquinones, such as compound A are being investigated for their electronic properties, e.g., conductivity (Angew Chem Int Ed, 2017, 56, 1). Answer the following questions about the structure of compound A.

(a) How many delocalizable electron pairs? (hint: it’s an even number)

(b) How many units of unsaturation? (hint: it’s an even number)

(c) Hybridization for either of the nitrogen atoms?

(d) Observable geometry for either of the nitrogen atoms?

(e) Electronic geometry for any of the sulfur atoms?

For geometrical labels, use complete words (e.g., “linear”) rather than abbreviations (e.g., “lin.”); write “n/a” if not observable.

Here is a question from Chapter 3 (3.35) - Your question: what is the molecular formula of NAAG?

What is the structure of the reaction product between NAAG (one of the most prevalent neurotransmitters in mammals) with excess aqueous sodium carbonate (give the molecule, derived from NAAG, including any necessary counterions)?

And finally, a question from an early draft of Chapter 1 that did not make the cut!

Under the reaction conditions, intermediate G goes on to produce N-formyl-monomethylhydrazine (N-formyl-MMH) and a byproduct H. The chemical equation is balanced; that is, the atoms in intermediate G are accounted for, exactly, by the atoms in N-formyl-MMH and byproduct H, both of which have rational organic chemical structures (all closed shell and uncharged atoms). Using the information given here and some logic, what is the structure of the byproduct (H)?
There are three fundamental principles of organic chemistry (and arguably, about chemistry in general):

1. The main group elements, particularly those in organic molecules, are "well-behaved" (bonding occurs in regular and predictable patterns).
2. In chemical reactions, atoms are conserved (so equations are balanced: the number and kind of atoms going in equals the number and kind of atoms coming out).
3. For the most part, chemical reactions are not explosions (that is, most of the structure of the molecules is maintained, and the reaction is a subtle change involving a few bonding changes rather than molecules flying apart and coming back together in completely new arrangements at each atom).

The main group elements are those in the "s" block and the "p" block, and organic molecules tend to involve mainly the subset outlined here (see table). By well-behaved, it means that a hydrogen atom in a molecule, when not bearing a charge, will invariably have one bond associated with it. For the second row p-block elements, it means that carbon atoms in molecules, when uncharged, will almost always have 4 bonds, nitrogen (and phosphorus) atoms will have 3 bonds and 1 non-bonding electron pair (nbe), oxygen (sulfur and selenium) will have 2 bonds and 2 nbe, and the halogens (fluorine, chlorine, bromine and iodine atoms) will have 1 bond and 3 nbe.

The predictable features of these atoms allow for the line abbreviation system that is used to represent organic molecules: carbon atoms can be represented as points, identifiable at the vertex of intersecting lines (bonds); atoms other than carbon and hydrogen ("heteroatoms") are shown, along with nbe as required; hydrogen atoms are included when the explicit atom label is used, but generally need not be shown for carbons when the "C" symbol is not used. The sooner a new student learning organic chemistry can subconsciously translate between these representational forms, no matter which one is being used, the better, as these line abbreviation drawings are the universal mode of communicating about the structural composition of organic molecules. Take, for example, these identical structures for \( \text{C}_4\text{H}_11\text{NO} \).

What is the molecular formula of this giant molecule, compound A? For now, ignore the rest.

Trichalcogenasumanene orthoquinones, such as compound A are being investigated for their electronic properties, e.g., conductivity (Angew Chem Int Ed, 2017, 56, 1). Answer the following questions about the structure of compound A.

(a) How many delocalizable electron pairs?
(b) How many units of unsaturation?
(c) Hybridization for either of the nitrogen atoms?
(d) Observable geometry for either of the nitrogen atoms?
(e) Electronic geometry for any of the sulfur atoms?
When posed with the questions (what are the molecular formulas for compound A, and for the NAAG molecule, the answer to the posed question needs to be identified as a translation. The process of translation cannot be uncovered in the question, nor the background knowledge. By answering the posed question the right away ("I need to do a translation"), you are then implicitly identifying what information you need to use to carry that out. After all, if you do not know that carbon and these other elements are well-behaved and predictable, you simply cannot figure that out from the information present - because that was not the question. The question is always this: to figure out the information you need to answer the posed question. On an exam, practically speaking, no matter how unfamiliar a question appears on the surface, it will represent one of the intended lessons, so you need to be able to understand/identify the question correctly before you can construct an answer.

**What is the molecular formula of this giant molecule?**

Whether you do it explicitly (by redrawing the entire structure) or implicitly (by imagining the atoms that are there), you need to be able to translate the line abbreviated structure into a structure with the atoms that are implied. This skill is absolutely one that needs to become second nature as rapidly as possible…

That process needs to be repeated over the entire structure - and it is at once immediately obvious why the line abbreviation system is used, but also why it is important to be mentally registering all of this information when you look at an abbreviated molecular structural drawing (because an experienced person is "seeing" this information automatically, and using it)

Even counting the atoms can require a strategy to ensure that you are not missing any as you try to keep track of them; mentally dividing the molecule into easily visually segregated units and tallying them up separately might be one useful way of developing the molecular formula (format = C<sub>x</sub>H<sub>y</sub> then alphabetical order)
Without reiterating the detail, exactly the same process used for compound A can be repeated on the NAAG molecule. Indeed, everything from your textbook, to the course pack, to the internet, and millions of pages of chemistry journal pages, are filled with line abbreviation structures of organic molecules, and so other molecules to practice with could not be easier to find.

The same decisions and background information are needed. The answer to the question “what is the molecular formula,” you learned from the previous question, means “redraw the structure with the atoms” (either literally or in your imagination) - and that requires the understanding about (a) do you understand the well-behaved nature of the main group atoms? (b) do you understand the generalizations about each atom in a structure? (c) do you understand how the line abbreviation system works?, and (d) do you understand how to apply all three of these to any organic molecule you see?

None of these things is referenced in the information provided, or this particular question, and yet knowing these things are, implicitly, the direct answer to the question. The structure that you draw and the corresponding molecular formula simply fall out of that understanding. In other words, if you do not know that these four things are required, or if you do not know how to use them, you cannot draw the corresponding structure correctly, and you cannot get to the correct molecular formula.

What is the molecular formula of NAAG?

The question is “what is the molecular formula?” and the unstated guideline (redraw the structure with the atoms explicitly shown, or do this in your imagination) is required to get there.

Redrawing the molecule correctly (literally or mentally), means knowing these four things:

(a) the well-behaved nature of the main group atoms
(b) the generalizations about each atom in a structure
(c) how the line abbreviation system works
(d) how to apply all three of these to any organic molecule

And if you know all four of these things, then and only then can you translate the abbreviated structure into its more explicit version:

And then and only then can you count the proper number of atoms and, provided you know the proper format of a molecular formula, you can then generate this:

\( \text{C}_{11}\text{H}_{16}\text{N}_2\text{O}_8 \)

If all you worry about is “seeing the answer” or “checking the answer” against your proposed solution, how can you understand what part(s) of this process you did not understand (if you do not have the same solution) or, more diabolically, if you got the same solution by making a couple of errors that happened to cancel one another?

Successful learners are explicit with themselves about the steps they take, and they tend to enter into those conversations with others as in-depth explanations. As you can see in these two examples: once you learn how to do a process correctly, there is no comparable question that you cannot answer. Organic chemistry is filled with general principles that can be applied to hundreds of thousands of new examples that you have never seen before.
And finally, a question from an early draft of Chapter 1 that did not make the cut!

Under the reaction conditions, intermediate G goes on to produce N-formyl-monomethylhydrazine (N-formyl-MMH) and a byproduct H. The chemical equation is balanced; that is, the atoms in intermediate G are accounted for, exactly, by the atoms in N-formyl-MMH and byproduct H, both of which have rational organic chemical structures (all closed shell and uncharged atoms). Using the information given here and some logic, what is the structure of the by-product (H)?

\[
\text{intermediate G} \quad \xrightarrow{\text{under the reaction conditions}} \quad \text{N-formyl-MMH} + \text{byproduct H}
\]

At this point in CHEM 210, you do not have any chemically based knowledge to draw from about the reactivity of organic molecules, but you do have the three principles:
(a) these atoms are well-behaved
(b) atoms are conserved (balanced) in a chemical reaction
(c) most reactions are not explosions, and only involve subtle rather than dramatic changes

There is no exact process for answering this question, but, in fact, all three principles are required.

A first strategy might always be to inventory the atoms (principle b) because it simply involves counting. Depending on your comfort level with the line abbreviation formulas, you might want to redraw these into their translated structures to count the atoms (yes, using exactly the same process as the previous two questions!).

\[
\text{intermediate G} \quad \text{N-formyl-MMH}
\]

Applying principle b, after getting the translation correct, the molecular formula for byproduct H is \( \text{C}_2\text{H}_2\text{O}_2 \).

So, what is the structure? Principle c is next. Changing as little of the bonding as possible is the best option for identifying the possible structure. I can see in N-formyl-MMH that a considerable amount of the structure from intermediate G has been retained. The N-C bond has been broken, and replaced by a N-H bond, meaning that one of the Hs from the right hand side of the molecule (see arrows, below) ends up disconnected and reconnected. And sure enough, the remaining atoms are \( \text{C}_2\text{H}_4\text{O} \).

\[
\text{intermediate G} \quad \xrightarrow{\text{under the reaction conditions}} \quad \text{N-formyl-MMH} + \text{byproduct H}
\]

Which of the Hs is it? There is no way to tell (yet), so you need to consider that there are three uniquely different Hs over on the right hand side of the structure: the one on the oxygen, the one of the carbon attached to the nitrogen, and one of the three that are on the other carbon. I know it must be one of these Hs (principle b) but I do not know which one. Mentally, or by drawing them, I need to consider all three possibilities.
Under the reaction conditions, intermediate G goes on to produce N-formyl-monomethylhydrazine (N-formyl-MMH) and a byproduct H. The chemical equation is balanced; that is, the atoms in intermediate G are accounted for, exactly, by the atoms in N-formyl-MMH and byproduct H, both of which have rational organic chemical structures (all closed shell and uncharged atoms). Using the information given here and some logic, what is the structure of the by-product (H)?

All three options are shown. Thus, using principle c, each of the three unique Hs is disconnected in three distinctive cases (A, B, and C), and reconnected to give N-formyl-MMH, and all of which leave a C$\textsubscript{2}$H$_4$O segment remaining.

Finally, principle c and principle a are needed, in combination. None of these C$\textsubscript{2}$H$_4$O segments are rational structures, according to the rules for the well-behaved atoms. In Case A, the oxygen and its appended carbon are both incomplete, but they can be completed by creating a double bond between them. In Case B, the two carbons are incomplete, but they can be completed by creating a double bond between them. In Case C, however, only the one carbon is incomplete, and the only way to solve that is to start disconnecting and reconnecting other atoms, which is against principle c.

And, yes: this problem has two perfectly consistent and equally valid solutions. Real science is like that.