6.4: THE WHAT- WHAT WERE THE MAJOR FINDINGS OF THE EXPERIMENT?

Section 5. Data

(1) General: Data that you collect must be presented clearly. In almost all cases, a tabulated form is required. The data that you should present is intimately tied to the purpose of the experiment. If the purpose is to synthesize a compound, the data are related to that purpose, i.e. they indicate whether or not the synthesis was successful.

Tables should be numbered and have captions. Units should be given in the title cells, in parentheses or brackets.

Most likely, the data will be analytical and spectroscopic data. Examples are:

- **TLC-analysis (spots, distance travelled, Rf-values),**
- **Melting point data (melting point ranges, literature values)**
- **IR-spectroscopy data (functional groups, wavenumber, literature values)**
- **Synthesis data (only appropriate when a chemical synthesis has been performed): masses, volumes (if applicable), densities (if applicable), moles, yields**
- **NMR data (assignment, shift values, integrals)**

In each table, the most important data should be presented. The task is to filter out the important data points. For example, when providing a table with IR data, you can readily find many peaks, but most of them are irrelevant to the purpose of an experiment or do not provide any information about the success of the experiment

A key task is therefore to select and present meaningful data, and not just dump all your data into the report.

If you have acquired an IR (or NMR) spectrum, a copy of the spectrum should be included in this section.

(2) Things to watch out for: Two common examples of irrelevant data include mass of glassware and mass of filter paper. Appearance, consistency of a product and other physical properties of a similar nature, are also inappropriate. Make sure that the tables are formatted correctly.

(3) Some examples:

Good Table:

Table 1. Synthesis table

Compound	Mw, [g/mol],	m, [g],	n, [mmol],	Yield, [%],
Benzaldehyde	182	0.21	1.2	-
$NaBH_4$	38	0.10	2.6	-
1,1-diphenylmethanol	184	0.19	1.0	83

Good Table:

Table 2. IR data

Bond	Observed value [cm-1]	Literature value [cm-1]
O-H	3550	3200-3600
C-H (sp^2)	3010	3090-3005
C-H (sp^3)	2985	2985-2800

SECTION 6. INTERPRET THE OBTAINED RESULTS (OR WHAT DID YOUR DATA MEAN?)

(1) General: In many cases, interpretation of data is the most challenging component of any report. The key feature of an interpretation is that it says something about the data that relates to the purpose of that experiment.

There are two important scenarios: If the purpose of the experiment is to identify an unknown sample, then the interpretation extract information from the data that says something about the identity of the unknown. If the purpose of the experiment is to synthesize a compound, the interpretation must extract information that describes the identity and purity of the target compound.

The natural tendency is to write interpretations that are far too long. A good interpretation is exact, precise, and addresses the purpose of the experiment.

Such information can be:

1. **TLC (says something about purity and identity)**
2. **Melting point (says something about purity and identity, especially when compared to a known melting point)**
3. **IR data (says something about which functional groups contained in the sample, which might indicate the presence or lack of the suspected product)**
4. **Yield (says something about the success of the reaction)**
5. **Boiling point (says something about the identity of the compound)**

Your data may not always support the expected outcome of an experiment. For example, your data may indicate that no reaction took place, or a product was very impure, and so on. These types of interpretations are appropriate as long as they are based on actual observations.

An example of a data interpretation that does not support the expected outcome is when you call attention to an OH peak in the IR spectrum that is not consistent with the structure of the desired product. That should be addressed, and a likely scenario to explain the presence of that peak should be provided.

(2) Things to watch out for: Unfocused or off-topic interpretations. Examples: interpretations that discuss what you learned, experiences you had or comments about your success as a lab student. None of these examples relates to the purpose of the experiment, and none of them deal with the objective data you collected. The interpretation should not deal with unimportant or irrelevant observations.

For example, if you say that the IR spectrum did not show the correct peaks because you collected the spectrum in a wrong way, that becomes a meaningless statement (how is it possible to collect a spectrum wrong, how do you know it is wrong, and why did you not address that issue if you knew about it?).

Here are some other examples with speculative conclusions that should be avoided.

- **I weighed something wrong, or the scales were wrong**
- **The yield was low because I transferred the sample between vials**
- **The glassware used has a high degree of uncertainty**

Furthermore, any error must have a direction and observations cannot contradict themselves.

If we come back to the example above with the OH peak that was found in your IR, that should not be there, surely that must mean that your yield also cannot be correct. And what about your melting point? That must also be off, or broader than it should be.

(3) Some examples:

Bad (imprecise, does not refer to specific data, no clear connection to the purpose of the experiment): The yield was higher than I wanted because of impurities and I weighed the sample wrong. The IR does not show what I should have because of something happening during the collection of the spectrum that should not have happened. The cylinder I used to measure was wet so that led to not getting correct data.

Bad (does not refer to any specific data, does not connect data to the purpose of the experiment, irrelevant):

IR spectroscopy is used to saying something about which functional groups are found in an organic mol- ecule. It can be used to find bonds that correspond to different functional groups. In my molecule, I have many bonds, and that can be seen in the spectrum. Furthermore, I have some strong peaks, and some weak ones, which is to be expected.

Good (Discusses specific data, interprets these data to support specific conclusion that relate to the pur- pose of the experiment): The yield was higher than expected (104%) due to alcohol contaminants in the isolated product. This is evident from the IR-spectrum of the sample (O-H stretch at 3551 cm^{-1}), which is a bond not present in the product. The melting point mirrors this (74.1°C - 84.9°C), as it is broader than expected (81.5-85.0°C)[1].

1. Correct citation to a literature source for the melting point.

SECTION 7. CONCLUSIONS (OR WHAT WAS THE PRIMARy RESULT OF YOUR EXPERIMENT)

(1) General: The conclusion will be the final statement based on the success (or lack thereof) in the experiment. It will pertain to the purpose of the experiment. It will draw on the interpretation under #6, and lead you to say something logical about the success

of the experiment as a whole.

Some points that often are relevant are:

- **Did you synthesize the suspected product (why, why not?)**
- **What was the purity of the compound isolated, what was the identity of the compound?**

(2) Things to watch out for: Conclusions that are not anchored in the purpose of the experiment should be avoided. If you have recrystallized a product, concluding about how much you liked or did not like the lab, is not appropriate. Subjective opinions and learning outcomes, although important to us, are not things that should be placed in the conclusion. Also, avoid using statements about what you would have done differently.

(3) Some examples:

Bad (irrelevant): I really liked learning about melting point analysis and I can see that it will be valuable for me in the future, because I am becoming a melting point expert.

Good (says something about the success of the experiment and its purpose): Benzoic acid was prepared in a moderate yield. The product isolated is likely benzoic acid, as it shows a similar IR spectrum that contains the key functional groups.
