AN EXAMPLE LABORATORY REPORT

by

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CHEMISTRY 446
Here you enter the section and group numbers.
EXPERIMENT 6

Here you insert the date that the report is submitted.

Abstract

The general format of a laboratory report is explained and illustrated. Each section is illustrated. Common errors and problems are discussed. Data analogous to those of experiment 6 are used to demonstrate a typical report structure. [NOTE: THE ABSTRACT SHOULD ALWAYS BE THE **LAST** SECTION ONE WRITES. IT IS A SUMMARY, WHICH CANNOT BE DONE UNTIL ALL OF THE WORK OF THE EXPERIMENT AND THE WRITING OF OTHER SECTIONS IS FINISHED.]

Text in blue font indicates text that is part of the report. Text is black is commentary on how to write the report.

Example Laboratory Report

1. Introduction

Writing a laboratory report is as important as taking data. When I say "writing," that includes the careful analysis of data and attention to the details of how the information is formatted for the ultimate reader. Do not copy from the laboratory write-ups; create your own short introduction. The introduction should be concise. It should explain the outlines of the experiment, what results have been determined, and salient points about the experiment. It should be about how your experiment worked, not some reprise of the general statements in the write-ups. Remember that an introduction "tells the reader what he/she is going to be reading." Here is an example of a concise introduction:

The infrared (IR) spectrum of CO has been analyzed to determine the fundamental constants of the molecule. The results can be expressed in terms of the rotation constant, B_e, the rotation-vibration constant, α_e, and the vibrational frequency. By IR spectroscopy on ground state molecules, it is not possible to determine the zeroth-order vibrational frequency, so we report the vibrational frequency, $\nu_0 - 2x_e\nu_0$. The results are consistent with data in the literature, within experimental error.

The object of the introduction is to give the reader a sense of what you are doing, why you are doing it in the way you are doing the experiment, and what results you have determined. Since scientific results are considered to be independent of the observer, it is appropriate to state any differences between one's work and that of others. It may be appropriate to give numbers at this point (as well as in a section labeled "Conclusions", but it is not always necessary.

2. Experimental

The section entitled "Experimental" generally contains information on the physical properties of the experiment, such as the type of instrumentation used, the variables controlled and those that are not controlled, and any unusual conditions. Here is an example of a section of that type.

The experiment was carried out with a Nicolet Fourier transform infrared (FTIR) spectrometer. The resolution of the spectrometer was set at 1 cm^{-1} for all spectra. The experiment involved the accumulation of background spectra which were subtracted from the spectra of the sample to provide the response of the sample. The detector was a nitrogen-cooled cadmium-telluride detector. Each experiment resulted from the average 64 transient responses coadded, with the background spectrum being the accumulation of 64 spectra without the sample present. The data were analyzed by Fourier transformation using the software of the instrument. The data were saved to disk, and were subsequently analyzed with a spreadsheet program, in this case, Microsoft EXCEL.

The section need not be long, but it should include everything about the experimental setup that the author thinks is important. While the data are usually gathered with an infrared spectrometer, the data discussed below are taken from Noggle's book.[1] In a real report, one would include such things as calibration of instruments and special features. In addition, in some cases it is

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[1] J. H. Noggle, *Physical Chemistry*, 3rd Edition, Harper-Collins, New York, 1996, p. 835. [NOTE THE FORMAT OF FOOTNOTES; THIS FORMAT SHOULD BE USED AT ALL TIMES.]

appropriate to discuss features such as how well the temperature was controlled (if it was or if it was necessary), barometric pressure or other pertinent experimental details such as concentrations of solutions (with an indication of calculations). Anything important in defining the experimental conditions should be stated. One should also report safety concerns in this section.

3. Results and Discussion

To start this section one has to refer to data. I do not write an example paragraph, but the student should be able to write out a simple explanation. In the case of the infrared spectrum, the data are the positions of absorptions read off the spectrum. In other experiments, there may not be a table of data. In some cases there may be plots of data. Note the format of a table. There is a title. Generally there is a heading for each column describing what is contained in the column (including the appropriate units), and there are entries below that. If you are using WORD or some similar word processing program, you may be able to format the table in different ways. Don't get carried away with this sort of thing; the important thing is to convey to the reader as precisely as possible what the data are. Do not allow the word processor to split a table unless there are so many entries that is absolutely necessary.

In writing each report, you have to make judgments about what things to include in the text of the report, sometimes original data, sometimes partially reduced data. Data must be accompanied by some estimate of the uncertainty. The exact form of the reported uncertainty depends on the data source. In this case, I assumed that the data were uncertain to 1 unit in the last reported digit. A difference, such as the second column, has a larger uncertainty by virtue of the rules for determining uncertainty. I show a footnote way and an in-line way; use only one.

TABLE I. PARTIAL LIST OF LINE POSITIONS IN THE SPECTRUM OF $^{12}C^{16}O$			
Line Position (cm^{-1})[a]	Line Position Difference (cm^{-1})[b]	J	J'
2115.632		7	6
2119.681	4.049 ± 0.002	6	5
2123.700	4.019 ± 0.002	5	4
2127.684	3.984 ± 0.002	4	3
2131.633	3.949 ± 0.002	3	2
2135.548	3.915 ± 0.002	2	1
2139.427	3.879 ± 0.002	1	0
2147.084	7.657 ± 0.002	0	1
2150.858	3.774 ± 0.002	1	2
2154.599	3.741 ± 0.002	2	3
2158.301	3.702 ± 0.002	3	4
2161.971	3.670 ± 0.002	4	5
2165.602	3.631 ± 0.002	5	6
[a] The uncertainty in the line position is ± 0.001 cm^{-1}. [b] The uncertainty in the difference is ± 0.002 cm^{-1}.			

Example Laboratory Report

Determining Associated Quantum Numbers

[NOTE THAT I CREATED A HEADING FOR THIS SUBSECTION TO MAKE IT CLEAR TO THE READER THAT I AM DISCUSSING SOMETHING SPECIAL. I DID NOT NUMBER THE SUBSECTION.]

Sometimes there are special considerations of data reduction. You should explain these clearly and concisely in a section of the results and discussion, as shown below.

One difficulty in resolving the data in the vibration-rotation spectroscopy experiment is determining the quantum numbers associated with each transition. For diatomic molecules, the J=0 ↔ J=0 transition is forbidden and will be absent from the spectrum. This makes the separation of the first transition of the R branch from the first transition of the P branch approximately twice the spacing of the other transitions (which are otherwise roughly equally spaced). Examination of the difference between the line positions (second column of Table I) reveals that the lines are not exactly equally spaced. In particular, the two transitions at 2139.427 cm^{-1} and 2147.084 cm^{-1} have a much wider separation than the others. It is reasonable to assign these two transitions to J=1→J'=0 and J=0→J'=1, one from the P branch and one from the R branch. Once that assignment is made, assigning J and J' for each of the other transitions is straightforward, since each transition corresponds to the rd and fourth rows of Table I.

Analyzing the Branches to Obtain Parameters

[NOTE THAT A NEW SUBSECTION IS STARTED BECAUSE THIS ANOTHER PHASE OF THE ANALYSIS.].

The energies of the transitions vary with either with J (P branch) or J' (=J+1, R branch). The determination of parameters requires an analysis of a plot of line position (or line-position difference) versus the appropriate quantum number. There are at least three different ways to do this. One may plot the energy of each transition versus quantum number. One may plot the difference of adjacent transitions as a function of the appropriate quantum number, or one may plot line differences between the two branches as a function of quantum number. The equations for each of these are derived from the equations in the write-up. The third method is often recommended. In principle, careful attention to detail should give results that are the same by any analytical protocol. Here is an example of what one might say in a report:

We decided to analyze the data by determining the coefficients in the predicted change in the line position. These are expected to follow equations (1), where *m* is either *J* or *J'* depending on the branch:

$$\Delta E_R = \omega_0 + B_1 m(m+1) - B_0(m-1)m$$
$$\Delta E_P = \omega_0 + B_1 m(m-1) - B_0 m(m+1) \qquad (1)$$

In this equation, the definitions of the parameters are as follows: *B*s are rotational constants for the vibrational states and $\omega_0 = \omega_e - 2x_e\omega_e$. Expansion of the first of these equations gives equation (2), a second-order equation in *m*:

$$\Delta E_R = \omega_0 + (B_1 + B_0)m + (B_1 - B_0)m^2. \qquad (2)$$

A similar equation can be found by expanding the second equation. From a plot of *ΔE_R* versus *m*, one determines the values of *B_1, B_0*, and *ω_0* from the best-fit coefficients. An EXCEL graph of the data is given in Figure 1, showing plots for the R and P branches.

Example Laboratory Report

In EXCEL, one may arrange to show the best-fit equation on the graph, and this is done in Figure 1. Note the correlation coefficient, which shows that these are excellent fits to the data. [NOTE: ALL FIGURES SHOULD BE NUMBERED CONSECUTIVELY THROUGHOUT THE REPORT. EACH FIGURE SHOULD HAVE A CAPTION BELOW IT THAT SHOULD CLEARLY STATE THE NATURE OF THE INFORMAITON IN THE FIGURE.]
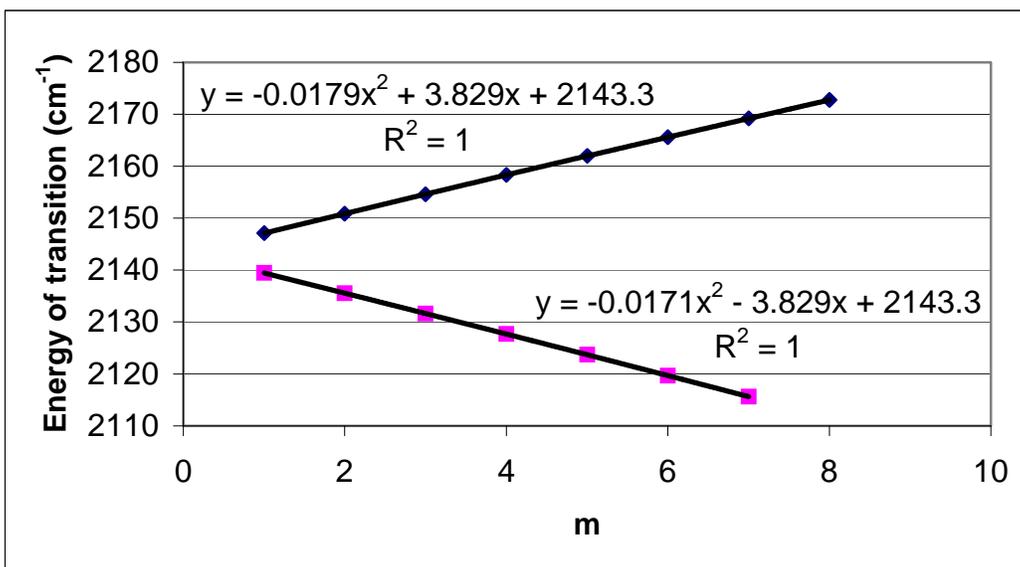

Figure 1. Plots of line-position differences versus m for the R and P branches of carbon monoxide.

In this case, these coefficients are not the final data to be reported. However, one can obtain the final values by algebra. Only the data from the R branch are shown below, but you should show both. So, the author would continue with the following paragraph.

The coefficients in these fits give values for the rotational and vibrational parameters of carbon monoxide by a simple algebraic transformation. The results for the R branch are given below:

R Branch:

$$\omega_0 = 2143.3 \ (\pm 0.1) \ \text{cm}^{-1}$$
$$B_1 + B_0 = 3.829 \ (\pm 0.001) \ \text{cm}^{-1}$$
$$B_1 - B_0 = -0.018 \ (\pm 0.001) \ \text{cm}^{-1}$$

These result in simultaneous equations for the parameters. Solving these gives:

$$B_1 = 1.905 \ (\pm 0.0014) \ \text{cm}^{-1}$$
$$B_0 = 1.924 \ (\pm 0.0014) \ \text{cm}^{-1}$$

Note that uncertainties are reported for each of these values. You would also report the analysis of the P branch as well in your report. Then the report would continue:

With these numbers, the equilibrium rotational constant and the rotation-vibration coupling constant are determined:

$$\alpha_e = B_0 - B_1 = 0.0179 \ (\pm 0.002) \ \text{cm}^{-1} \tag{3}$$

Example Laboratory Report

$$B_e = \text{½}(3B_0 - B_1) = \text{½}(3(1.924 \text{ cm}^{-1}) - 1.905 \text{ cm}^{-1}) = 1.933 (\pm 0.008) \text{ cm}^{-1}. \quad (4)$$

The data are summarized in Table II, along with values from the literature.

It is sometimes helpful to summarize results in a table.

TABLE II. SUMMARY OF RESULTS FROM INFRARED SPECTROSCOPY OF $^{12}C^{16}O$

Parameter	Experimental Value	Literature Value[a]
$\omega_e - 2x_e\omega_e$	$2142.2 \pm 0.1 \text{ cm}^{-1}$	2143.3 cm^{-1}
B_e	$1.933 \pm 0.008 \text{ cm}^{-1}$	1.9313 cm^{-1}
α_e	$0.018 \pm 0.002 \text{ cm}^{-1}$	0.01748 cm^{-1}
R_e	$0.1128 \pm 0.0007 \text{ nm}$	0.11281 nm
[a] From W. Gordy, W. V. Smith, and R. F. Trambarulo, *Microwave Spectroscopy*, Dover Publications, New York, 1953.		

The Bond Length

Again, note that I have added this as a separate subsection for clarity.

From knowledge of B_e, the parameter R_e can be calculated from the definition of the equilibrium rotation constant:

$$B_e = \frac{h}{8\pi^2 Ic}, \quad (5)$$

where I is the moment of inertia, c is the speed of light in a vacuum, and h is Planck's constant. Rearranging this equation, one calculates the moment of inertia of CO:

$$I = \frac{6.6260755 * 10^{-34} \text{ joule} - \sec}{8 * \pi^2 * 193.3 m^{-1} * 2.99792458 * 10^8 m/\sec} = 1.4489 * 10^{-46} kg - m^2$$

Since the uncertainty in the constants is much smaller than the uncertainty in the measured value of B_e, only the uncertainty in this latter quantity makes a significant contribution to the uncertainty in I. One may estimate this by percentage (about 1.3%), so the result for the moment of inertia is:

$$I = 1.4489 (\pm 0.019) \times 10^{-46} \text{ kg-m}^2.$$

To determine R_e requires knowledge of the reduced mass of $^{12}C^{16}O$. The exact masses of the two atoms can be found from standard references.[2] The values are

$$m_C = 0.012000000 \text{ kg, exactly}$$
$$m_O = 0.0159949146 \text{ kg},$$

with an assumed uncertainty of 1 in the last digit. From these, one obtains the reduced mass:

$$\mu = \frac{0.012 * 0.0159949146}{(0.012 + 0.0159949146) * 6.0221367 * 10^{23}} kg = 1.1385009 * 10^{-26} kg$$

Finally, the value of R_e can be calculated as:

$$R_e = \sqrt{\frac{1.4489038 \times 10^{-46} kg - m^2}{1.1385009 \times 10^{-26} kg}} = 1.1281 \times 10^{-10} m$$

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[2] For example, see Table 13.2 in J. H. Noggle, *Physical Chemistry*, 3rd Edition, Harper-Collins, New York, 1996.

Example Laboratory Report

One may show, if the uncertainty arises only from the determination of the moment of inertia, that:

$$\left|\frac{\Delta R_e}{R_e}\right| \;=\; \frac{1}{2}\left|\frac{\Delta I}{I}\right|. \tag{6}$$

so the percentage error is one half that for the moment of inertia, or 0.7%. So, the value of the interatomic distance is:

$$R_e = 0.1128\,(\pm\,0.0007)\ \text{nm}.$$

This compares favorably to the reported value of 0.11282 nm in Table II.

Theoretical Predictions of Parameters

The values of the various parameters were calculated using GAUSSIAN-98.[3] The calculation was carried out in a restricted Hartree-Fock model, using the 6-31G(d) basis set. First, the bond distance was optimized. From the data generated, a plot of energy versus bond length was constructed. [At this point you may wish to insert a figure that shows the variation of energy with bond length. Do not forget to reference the figure in the text.] From the variation of energy with bond distance, the optimal distance is found to be 0.11138 nm, not too different from the experimentally determined value. The program also predicts the rotational constant for this configuration, which in this case it gave as 59.4205597 GHz. Converting this to the standard units used throughout this report, $B_e = 1.982\ \text{cm}^{-1}$. Again, this is a little high, compared to the value determined experimentally.

In a second calculation, the harmonic frequency for this geometry was determined to be 2439.0288 cm^{-1}. In Table III, the experimental and theoretical results are summarized. One cannot experimentally determine the harmonic frequency from this experiment alone, so the experimental band center is given for comparison.

TABLE III. COMPARISON OF CALCULATED AND EXPERIMENTAL PARAMETERS FOR CARBON MONOXIDE		
Parameter	**Calculated with GAUSSIAN**	**Experimental**
R_e	0.1114 nm	0.1128 nm
B_e	1.982 cm^{-1}	1.933 cm^{-1}
ω_e	2439.0 cm^{-1}	
$\omega_e - 2x_e\omega_e$		2141.4 cm^{-1}

[3] Gaussian 98, Revision A.7, M. J. Frisch, G. W. Trucks, . B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrewski, H. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L . Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P. M. W. Gill, B, Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople, Gaussian, Inc., Pittsburgh, PA, 1998.

Example Laboratory Report

4. Discussion Questions

In this section, you write each of the discussion questions in order, immediately following each question by a brief answer. The length of the answer varies from question to question, and the length of this section varies from experiment to experiment.

5. Conclusions

You may include a section with your observations and comments. It is often convenient to reiterate the results in text form. Summarizing the laboratory experiment, including any problems that may have arisen, is a good practice.

5. References

You may include references in a separate section at the end of the report, rather than in footnote style, if you prefer. They would go at this point. Whatever you do, it is important that you be consistent. Do not use one style for part of a report and another for a later part of the report. Please use the American Chemical Society style for references. Do not hand in a report with only references to Internet sites.

6. Appendices

From report to report, it may be necessary to append various data and/or calculations. Include these at this point in the report.