Take-Home Assignment 1

On the course website you will find three spreadsheets that contain the raw digitized UV spectra for benzene collected from 240–290 nm using a double-beam, scanning spectrophotometer. Each spectrum was recorded for a different combination of three important instrumental variables: scan rate (in nm/sec), response time (in sec), and slit width (in nm). The spreadsheets are saved as .csv files, which you may, as you wish, open in Excel or in R. The table here summarizes the data by tab.

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| --- | --- | --- | --- | --- | --- | --- |
| file | scan rate | | response time[[1]](#footnote-1) | | slit width[[2]](#footnote-2) | |
| benzene\_slitwidth.csv | 20 nm/s | | 1 (0.1 s) | | 0.25 nm | 1.0 nm |
| 2.0 nm | 4.0 nm |
| benzene\_scanrate.csv | 5 nm/s | 10 nm/s | 3 (0.5 s) | | 1.0 nm | |
| 20 nm/s | 60 nm/s |
| 120 nm/s | 200 nm/s |
| 300 nm/s | 750 nm/s |
| 1500 nm/s | |
| benzene\_response.csv | 60 nm/s | | 1 (0.1 s) | 2 (0.2 s) | 1.0 nm | |
| 3 (0.5 s) | 4 (1.0 s) |
| 5 (2.0 s) | 6 (5.0 s) |
| 7 (10.0 s) | |

For the purpose of the questions that follow, assume the following set of conditions is the standard spectrum against which all other spectra are compared:

scan rate: 5 nm/s response time: 3 (0.5 s) slit width: 1.0 nm.

1. The standard UV spectrum for benzene, as defined here, has four identifiable peaks (three are obvious; the fourth appears as a shoulder on the high energy side of the spectrum). Report the wavelength and absorbance value for each peak.

2. For each variable—scan rate, response time, and slit width—how does a change in its value affect the spectrum. Consider issues such as signal-to-noise ratio, absorbance values for the four peaks identified in question 1, and shifts in the positions of peaks. Your answer to this question should be in the form of a well-written set of paragraphs illustrated with appropriate figures and/or tables.

3. Given you answer to the previous question, how might you balance the competing interests of analysis time, wavelength accuracy, and absorbance accuracy. Propose a set of conditions that will produce a spectrum with acceptable accuracy in absorbance and peak position with a short analysis time. Defend your choice of conditions in a single well-written paragraph. Be sure to explain your reasoning. Please note that this question calls for a subjective judgment; there is no correct answer to this question (although there are stronger and weaker answers).

This assignment is due in class next Monday.

1. The instrument setting for response time is a dial with values from 1 to 7. The values in parentheses are the actual response times in seconds. [↑](#footnote-ref-1)
2. Slit widths are reported as the effective bandpass in nm. [↑](#footnote-ref-2)