

## CHEM 454L – Excel Exercise 2

### Matrix Manipulation

- 1 Open a new spreadsheet in Excel.
- 2 In column A, starting with cell A1, enter the numbers 1, 3, 2, and 1, respectively.
- 3 Likewise, in column B enter the numbers 6, 16, 24, 15; in column C the sequence 4, 10, 13, 4; and in column D the numbers 4, 14, 17, and 8.
- 4 The resulting array should occupy the block A1:D4, and look like this:

|   |    |    |    |
|---|----|----|----|
| 1 | 6  | 4  | 4  |
| 3 | 16 | 10 | 14 |
| 2 | 24 | 13 | 17 |
| 1 | 15 | 4  | 8  |

This will be our test array, a 4 x 4 matrix.

- 5 Matrix inversion. In order to invert this matrix, we first select a location for its inverse, by selecting the top left corner cell of where you want the inverse to appear, say F1.
- 6 Highlight the space required for the result. The inverse of a 4 x 4 matrix is also a 4 x 4matrix, so in this example you need to highlight the block F1:I4.
- 7 Type = MINVERSE(A1:D4) but *don't* press the Enter key yet.
- 8 Now hold down the Control and Shift keys, and with both of these down press the Enter key. That will do it: you should see the inverse in block F1:I4.

- 9** Matrix multiplication. Now multiply the two matrices we already have on the spreadsheet. Since one is the inverse of the other, their product should of course be the unit matrix. The procedure is analogous to that of steps (5) through (8).
- 10** Go to the left top corner of where you want the product to appear, say A6. Highlight the required area, say A6:D9. Type = MMULT(A1:D4,F1:I4), and hold down Ctrl + Shift while depressing Enter.
- 11** You should have obtained the unit matrix, although the zeros may have some round-off errors, though typically less than  $\pm 10^{-15}$ .
- 12** Verify that the product F1:I4 times A1:D4 also yields the unit matrix by calculating that product in F6:I9.
- 13** Note that the spreadsheet deals with arrays as entire blocks rather than with individual cells. This is perhaps best illustrated by trying to erase *part* of an array. Highlight A6:D8 and press Delete. Nothing will be deleted; instead you will get an error message, “Cannot change part of an array”. **Print this error message (whole screen) and turn in with answers.** Acknowledge the message box and highlight A6:D9. Now you will have no problem erasing it.

- 14** The determinant. This is an easy one, because the determinant of a matrix is a scalar (a single number) so you need not use the Ctrl + Shift + Enter trick. Just go to any empty cell, deposit the instruction = MDETERM(A1:D4) and (yes) press Enter. The answer, -196, will appear. How was it?
- 15** Try the same for the determinant of F1:I4. Then multiply the two determinants: their product should be 1.

In summary, only for matrix inversion and multiplication do you need to highlight the entire block where the result should appear, and then enter the instruction while holding down Ctrl + Shift.

**Note: Put answers for Instructions 4, 7, 8, 10, 11 and 14-5 on a single spreadsheet and turn in on Monday April 11. Don't forget to include your error message screen from Instruction 13.**

Exercise adapted from: How to Use Excel in Analytical Chemistry and in General Scientific Data Analysis by Robert de Levie, Cambridge University Press.