

Errata- Applying Maths in the Chemical and Biomolecular Sciences

Note: In some of the Maple algorithms the left dashes such as ` , a pair of which are used to enclose a name, have been printed as right dashes or ´.

Page 14, Algorithm 14.1 Recursive calculation of the experimental function

Read the following:

‘for i from 1 to 30 by 2 do’ as ‘for i from 1 to 30 do’ or ‘for i from 1 to 30 by 1 do’

Page 27

Change ‘Recurrence’ to ‘Recursion’ in the heading to Section 1.8.1 and also in the next line

Page 27, Algorithm 1.5 Recursive calculation of factorials

Read the following:

```
> m:= 6:
    n:= 1;
    for I from 1 to m-1 do
        n:= n*(i+1);
        print(I, n);
    end do:
```

where n returns the factorial. If you want a ‘pretty’ output, print using the instruction

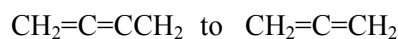
```
printf(" %d %g\n", I , n);.
```

Page 179

In Q 4.76, three lines from the end change ‘ α ’ to ‘a’.

Page 339

In the D_{2d} box change



Page 360

Two lines up from the bottom of the page change

`Phi := -40: to phi:= - 40:`

Page 368

On the last line, the reference to equation 6.18 should be to 7.18

Page 370

Five lines from the bottom of the page change ‘ w cm⁻²’ to ‘ W cm⁻²’.

Page 375

Three lines down delete ‘or y,’.

Page 422

In the last three lines at the bottom of the page change

`Anst to Angst`

Five lines from the bottom of the page change

`amu:= 1.667e-27 to amu:=1.660e-27`

Page 430

In Algorithm 8.1 line 4 change

`-hbar^2/(2*mu) to -hbar^2/(2*mu)`

and on line 7 change

`(-hbar^2 /(2*mu) to -hbar^2/(2*mu)`

Page 605 & 606

The three similar print statements in Algorithms 11.2, 11.3 and 11.4 should have left facing brackets and each statement should read

`print(`root` = xm, `function value` = f(xm));`

Page 606

In Algorithm 11.4, line 2 change

`xs:= to xm:=`

Page 621

In the middle of the page change

`Euler[i]` to `Eulery[i]`

to be consistent with Algorithm 11.9.

Page 630

In the heading to Algorithm 12.3 change

$p(x) = ke^{-kx}$ to $p(x) = e^{-kx}$

Page 655

In Algorithm 11.17 line 5, change

`dydx := (y, z) -> z;` to `dydx := z -> z ;`

Page 677

Eight lines from the top of the page change

`ln(events)` to `ln(A0)`

Page 691

If values of Boltzman's constant k_B and J are used that are different from 1 then the calculation of C_v in the last line of Algorithm 12.9 (page 692) should be changed according to the equation given on page 691. This can be conveniently done by defining k_B and T separately and then redefining `kBT` as `kBT := kB*T;`

Page 733

Two lines from the bottom of the page delete `m := nops(xval)`

Page 734

In the line above the figure, change

`dat_points` to `data_points`

The instructions to plot the calculated line was omitted and could be added as

`p3:=plot(line(x),x=0..25):` and this line plotted with the data using `p2:=plot([data_points], etc):` and the `display(p2,p3);` command; see the

Maple code in the online resource.