Key for Take-Home Assignment 03

This problem provides practice in writing a set of reactions for an acid–base equilibrium syste. Your neatly worked solutions to this problem is due at the end of this week.

In the last take-home assignment you drew a ladder diagram for glutamic acid, a triprotic amino acid with pK_a values of 2.233, 4.42, and 9.95 for the equilibria between the forms H_3A^+, H_2A, HA^-, and A^{2-}, where H_2A is its neutral form. Write a set of equations that describe completely a solution of 0.10 M H_2A. Using R or Excel, what is the pH of this solution? As a supplement to your written solution, please email me a copy of the R script or the spreadsheet you used to calculate the pH.

Answer

```
# provide equilibrium constants for all reactions
Kw = 1.00e-14
Ka1 = 5.9e-3
Ka2 = 3.8e-5
Ka3 = 1.12e-10

# provide total concentration for all mass balances
C = 0.1

# set up master variable
pH = seq(1, 14, 0.01)

# calculate concentrations of all species in system
H3O = 10^-pH
OH = Kw/H3O
HAnum = OH - H3O
HAden = H3O^2/(Ka1*Ka2) - 1 - 2*Ka3/H3O
HA = HAnum/HAden
A = Ka3 * HA/H3O
H2A = H3O*HA/Ka2
H3A = H3O*H2A/Ka1

# define error function using abolute value
error = abs(C - H3A - H2A - HA - A)

# find the index for the minimum error (the error closest to zero)
id = which.min(error)
id
```

```
## [1] 235
```

```
# report out all values
pH[id]
```

```
## [1] 3.34
```

```
H3O[id]
```

```
## [1] 0.0004570882
```

```
OH[id]
```

```
## [1] 2.187762e-11
```

```
H3A[id]
```

```
## [1] 0.006253841
```

```
H2A[id]
```

```
## [1] 0.08072328
```

```
HA[id]
```

```
## [1] 0.006710926
```

```
A[id]
```

```
## [1] 1.644373e-09
```

```
error[id]
```

```
## [1] 0.006311948
```

```
# plot of error function (if of interest)
plot(pH, log10(error), type = "l")
```