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Prelab

Experiment 6 Determination of the Mean Aggregation Number of a Micellar a System

Introduction

In this experiment will be determined the mean aggregation number of sodium dodecyl sulfate within micelles in aqueous solution. A fluorescence probe technique will be employed in the determination process.

To overcome the low solubilities of hydrocarbons these molecules, which have both hydrophobic and hydrophilic properties, are used. SDS; sodium dodecyl sulfate represents one of them which is broadly used in detergents and other surfactants.

When these molecules dissolve in water they have the tendency to change the bulk properties (such as surface tension) of the water molecules. The concentration, which these several properties are changed, is called CMC (critical micelle concentration). Above this concentration other roughly spherical shaped structures, which are called micelles, are formed.

N, the mean aggregation number is assumed to be the definite number of surfactant molecules.

Experimental

The experimental procedure is exactly how it is described in the lab manual.

Following the experiment, the average micelle concentration will be determined by using the equation

$[M]=([S_0])-CMC)/N$

where N is the mean aggregation number and CMC is the concentration of free monomers in solution, $[S_0]$ is the assumed bulk concentration of the surfactant molecule.

Fluorimetric technique will also be exposed to the students during this experiment. In this process a luminiscent probe molecule will be added to the micellar system and there will be more micelles present than probe molecules so that a micelle is either empty or associated with a probe molecule.

Then finally by using a linear least squares fit CMC and N can both be find by using the equation :

$\ln(I^o/I)=[Q]N/([S_0])-CMC)$

where I is the intensity of luminisence intensity, [Q] is the bulk quencher concentration. At the end the results will be compared with the theoratical values and the sources of error will be discussed.

Error Analysis

Miscalibrated laboratory equipment and inaccurate preparations of solutions could have significant effect in the error. The preparation of solutions and the recording of the temperature have to be done carefully to estimate the uncertainties more clearly.

Question -1.5
Units -0.5
Calcs -1
table -0.5

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Experiment 6 Determination of the Mean Aggregation Number of a Micellar a System

Abstract

The mean aggregation number of sodium dodecyl sulfate was calculated within micelles in aqueous solution using the fluorimetric technique. The CMC were found to be 0.9423±0.2M. The mean aggregation number, N were determined to be 2.502±0.16. what about N from the other part, 2 N values should be reported.

Introduction

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Discussion and Conclusions :

For part 1 the appropriate concentrations and the Q's are calculated and put in the table. To get a better result the intensities were taken twice and the average was used. Although the absorbance has to be same for all results there exists a slight error. Then the linear squares fit of first data were plotted and the slope and the intercept was found to be 4.55±0.67 and 0.018±0.047 respectively.

			PART 1			
A	0mL	2mL	4mL	6mL	8mL	10mL
B	10mL	8mL	6mL	4mL	2mL	0mL
Absorbance	1.2319	1.2141	1.2504	1.2130	1.1616	1.1722
Iavg	40.0	42.45	43.05	56.55	57.05	66.20
units Q[i]	0.1154	0.0926	0.06902	0.04616	0.02308	0
I[o]/I[i]	1.655	1.5594	1.5377	1.1706	1.1603	1
ln(I[o]/I[i])	0.5041	0.4443	0.4302	0.1575	0.1487	0

I^{o}

For the second part the S's are calculated, and for this part also the absorbances had to be equal but in fact there also a slight error existing. Then Iavg's were calculated and S[i] vs. 1/ln(I[o]/I[i]) data was plotted by using the linear squares fitting. The appropriate slope and the intercept were found with the errors. They are : 0.6158±0.13 and 0.5802±0.065 respectively.

		PART 2			
A	1mL	2mL	4mL	6mL	8mL
B	9mL	8mL	6mL	4mL	2mL
Absorbance	1.1273	1.287	1.1755	1.2544	1.2842
Iavg	65.9	60.05	59.65	56.45	46.45
units S[i]	0.6633	0.60564	0.49028	0.3749	0.25956
I[o]/I[i]	1	1.0974	1.1047	1.1674	1.4187
1/ln(I[o]/I[i])	1	0.9112 10	~~0.9030~~ 9.6	~~0.8566~~ 6.27	~~0.7048~~ 2.8

Following the calculation of slopes and the gradients N, CMC, Q and S were determined using the calculations at the end of the report. this is needed to calculate but I did not find your values.

Error Analysis

Miscalibrated laboratory equipment and inaccurate preparations of solutions had significant effect in the

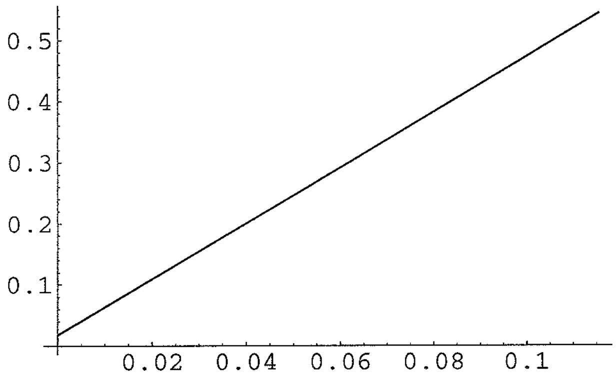
Where did you get these numbers?
$1/\ln[66.2/65.9] = 220$

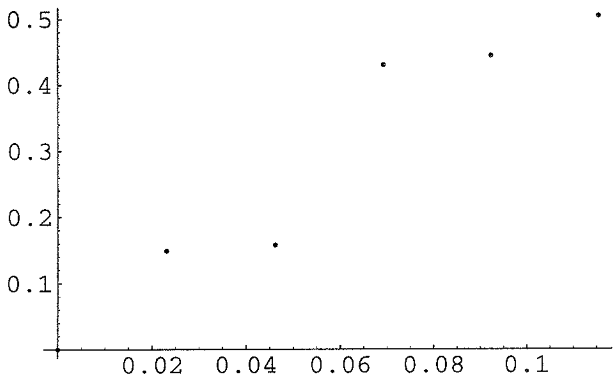
-0.5

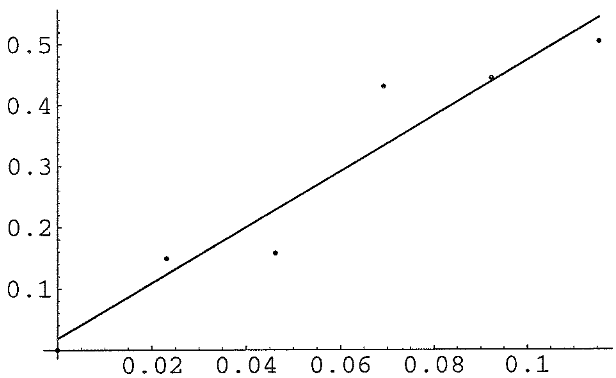
what temp did you record?

error. The preparation of solutions and the recording of the temperature were done carefully to estimate the uncertainties more clearly. The mean of the absorbances for the first one was 1.2072 with a standart deviation of 0.034 and the second one with 1.2257 with a standart deviation of 0.071. The logaritmic values of intensity ratios in Turro Yekta are much higher then what was found in the experiment these can be explained by the inaccurate preparations of the solutions.

```
In[1]:= (* To "run" a line, put the cursor on it, and press Shift-Enter *)
        (* You can also use a menu command to evaluate the whole notebook: Menu: Kernel →
          Evaluation → Evaluate Notebook *)

In[2]:= Needs["Statistics`LinearRegression`"]

In[3]:= $Packages

Out[3]= {Statistics`Common`MultivariateCommon`, Statistics`Common`RegressionCommon`,
         Statistics`Common`PopulationsCommon`, Statistics`ConfidenceIntervals`,
         Statistics`Common`DistributionsCommon`, Statistics`DescriptiveStatistics`,
         Statistics`NormalDistribution`, Statistics`LinearRegression`, Global`, System`}

In[4]:= (* Input your data;
         I am using the data from Table 8.1 in Taylor: "Intro to Error Analysis" *)

In[5]:= x[1] = 0.1154;
        x[2] = 0.0923;
        x[3] = 0.0692;
        x[4] = 0.04616;
        x[5] = 0.02308;
        x[6] = 0;
        y[1] = 0.5041;
        y[2] = 0.4443;
        y[3] = 0.4302;
        y[4] = 0.1575;
        y[5] = 0.1487;
        y[6] = 0;

        (* The next line refers to the number of points.  So,
         if you had 7 data points, numPoints=7 *)

In[17]:= numPoints = 6;

In[18]:= datatemp = Table[{Table[x[i], {i, 1, numPoints}], Table[y[i], {i, 1, numPoints}]}];
         data = Transpose[datatemp]

Out[18]= {{0.1154, 0.5041}, {0.0923, 0.4443},
          {0.0692, 0.4302}, {0.04616, 0.1575}, {0.02308, 0.1487}, {0, 0}}

        (* The next line does a fit *)

In[19]:= Regress[data, {1, x}, x, RegressionReport → {ParameterTable, RSquared, AdjustedRSquared}]

                                   Estimate     SE          TStat      PValue
Out[19]= {ParameterTable → 1       0.0179806    0.0471684   0.3812     0.722437   ,
                           x       4.55572      0.675115    6.74806    0.00251411
          RSquared → 0.919251, AdjustedRSquared → 0.899064}

In[20]:= (* The following line is used to print out plots.  See 3rd plot *)

In[21]:= g1 = Fit[data, {1, x}, x];

In[22]:= Show[
          Plot[g1, {x, Min[Table[x[i], {i, 1, numPoints}]], Max[Table[x[i], {i, 1, numPoints}]]}],
          ListPlot[data]]
```







Out[22]= - Graphics -

```
In[23]:= (* Comparison with Taylor: Equations 8.10, 8.11, 8.12, 8.15, 8.16, 8.17 *)

In[26]:= SumX = Sum[x[i], {i, 1, numPoints}]; SumXX = Sum[x[i]^2, {i, 1, numPoints}];
         SumY = Sum[y[i], {i, 1, numPoints}]; SumXY = Sum[x[i] * y[i], {i, 1, 5}];
```

In[27]:= $\Delta = 5 * \text{SumXX} - \text{SumX}^2$

Out[27]= 0.0266297

In[28]:= $\text{A} = \dfrac{\text{SumXX} * \text{SumY} - \text{SumX} * \text{SumXY}}{\Delta}$

Out[28]= 0.0377565

In[29]:= $B = \frac{5 * SumXY - SumX * SumY}{\Delta}$

Out[29]= 4.322

In[30]:= $SigmaY = \sqrt{\frac{1}{3} * Sum[(y[i] - A - B * x[i])^2, \{i, 1, 5\}]}$

Out[30]= 0.0737384

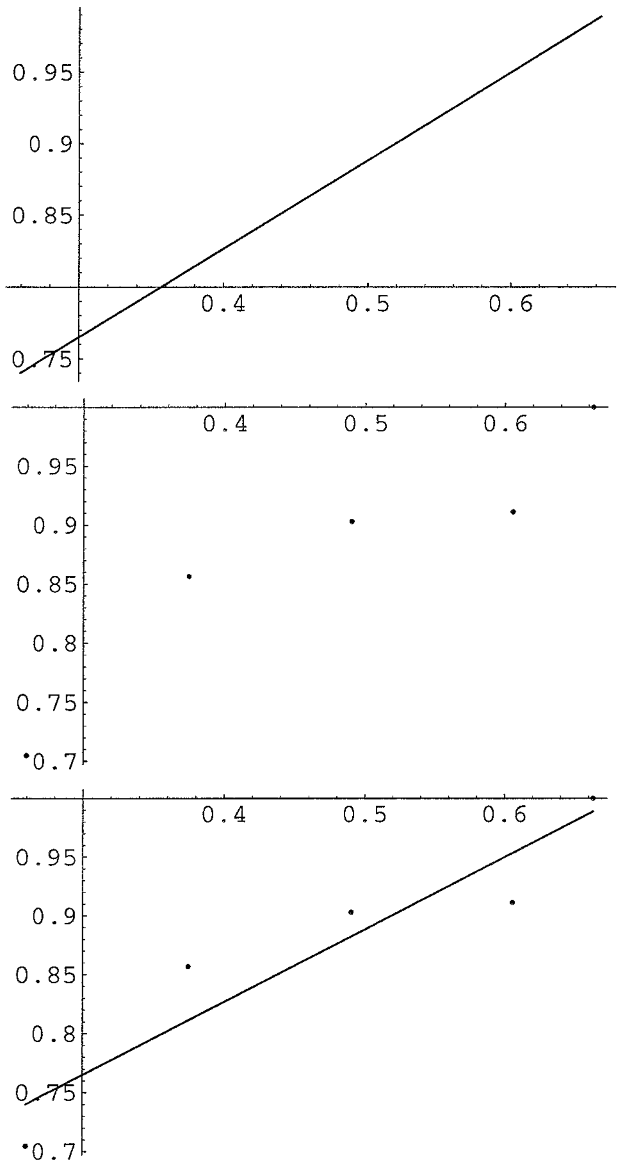
In[31]:= $errorInA = SigmaY * \sqrt{\frac{SumXX}{\Delta}}$

Out[31]= 0.077332

In[32]:= $errorinB = SigmaY * \sqrt{\frac{5}{\Delta}}$

Out[32]= 1.01041

```
In[33]:= (* To "run" a line, put the cursor on it, and press Shift-Enter *)
         (* You can also use a menu command to evaluate the whole notebook: Menu: Kernel →
           Evaluation → Evaluate Notebook *)

In[34]:= Needs["Statistics`LinearRegression`"]

In[35]:= $Packages

Out[35]= {Statistics`Common`MultivariateCommon`, Statistics`Common`RegressionCommon`,
          Statistics`Common`PopulationsCommon`, Statistics`ConfidenceIntervals`,
          Statistics`Common`DistributionsCommon`, Statistics`DescriptiveStatistics`,
          Statistics`NormalDistribution`, Statistics`LinearRegression`, Global`, System`}

In[36]:= (* Input your data;
          I am using the data from Table 8.1 in Taylor: "Intro to Error Analysis" *)

In[37]:= x[1] = 0.6633;
         x[2] = 0.60564;
         x[3] = 0.49028;
         x[4] = 0.3749;
         x[5] = 0.25956;
         y[1] = 1;
         y[2] = 0.9112;
         y[3] = 0.9030;
         y[4] = 0.8566;
         y[5] = 0.7048;

In[47]:= (* The next line refers to the number of points.  So,
          if you had 7 data points, numPoints=7 *)

In[48]:= numPoints = 5;

In[49]:= datatemp = Table[{Table[x[i], {i, 1, numPoints}], Table[y[i], {i, 1, numPoints}]}];
         data = Transpose[datatemp]

Out[49]= {{0.6633, 1}, {0.60564, 0.9112}, {0.49028, 0.903}, {0.3749, 0.8566}, {0.25956, 0.7048}}

In[50]:= (* The next line does a fit *)

In[51]:= Regress[data, {1, x}, x, RegressionReport → {ParameterTable, RSquared, AdjustedRSquared}]

                                   Estimate    SE           TStat      PValue
Out[51]= {ParameterTable → 1       0.580293    0.0657615    8.82421    0.00306705,
                           x       0.615844    0.131258     4.69188    0.0183065

          RSquared → 0.880066, AdjustedRSquared → 0.840088}


In[52]:= (* The following line is used to print out plots.  See 3rd plot *)

In[53]:= g1 = Fit[data, {1, x}, x];

In[54]:= Show[
          Plot[g1, {x, Min[Table[x[i], {i, 1, numPoints}]], Max[Table[x[i], {i, 1, numPoints}]]}],
          ListPlot[data]]
```



Out[54]= - Graphics -

In[55]:=
```
(* Comparison with Taylor: Equations 8.10, 8.11, 8.12, 8.15, 8.16, 8.17 *)
```

In[56]:=
```
SumX = Sum[x[i], {i, 1, numPoints}]; SumXX = Sum[x[i]^2, {i, 1, numPoints}];
SumY = Sum[y[i], {i, 1, numPoints}]; SumXY = Sum[x[i] * y[i], {i, 1, 5}];
```

In[57]:= $\Delta = 5 * \mathrm{SumXX} - \mathrm{SumX}^2$

Out[57]= 0.545609

In[58]:= $A = \dfrac{\mathrm{SumXX} * \mathrm{SumY} - \mathrm{SumX} * \mathrm{SumXY}}{\Delta}$

Out[58]= 0.580293

In[59]:= $B = \frac{5 * SumXY - SumX * SumY}{\Delta}$

Out[59]= 0.615844

In[60]:= $SigmaY = \sqrt{\frac{1}{3} * Sum[(y[i] - A - B * x[i])^2, \{i, 1, 5\}]}$

Out[60]= 0.0433591

In[61]:= $errorInA = SigmaY * \sqrt{\frac{SumXX}{\Delta}}$

Out[61]= 0.0657615

In[62]:= $errorinB = SigmaY * \sqrt{\frac{5}{\Delta}}$

Out[62]= 0.131258

- Calculations -

Part 2

$x = 0.6158$ $\sigma_x = 0.131$

$b = 0.5802$ $\sigma_b = 0.065$

$$CMC = \left|\frac{-b}{m}\right| = \underline{0.9423} \text{ units}$$

$$\sigma_{CMC} = \sqrt{\frac{b^2\sigma_x^2 + \sigma_b^2 \cancel{x}^2}{x^4}}$$

Where are your calculations for the other N value? (-1)

$$\sigma_{cmc} = \underline{0.2275} \text{ units}$$

$S = 0.6489$ ~~units~~

$$N = \frac{1}{\theta_1 \cdot m}$$

what is this value?

$$= \underline{2.502}$$

$$\sigma_N = \sqrt{\frac{\sigma_q^2 \cancel{x}^2 + \sigma_x^2 \theta^2}{x^4 \theta^4}}$$

$$= \frac{(0.025^2 \cdot 0.6158^2) + (0.1312)^2(2.502)^2}{(0.6158)^4(2.502)^4} = \underline{0.16}$$

Part 1

$x = \cancel{0.0179}\ 4.595$ $b = 0.01798$

$\sigma_x = 0.675$ $\sigma_b = 0.04716$