Partial Molal Volume

CHEM 445 - 025L

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ABSTRACT

The partial molal volumes for glycine, β-alanine, γ-aminobutyric acid (GABA), and 6-aminohexanoic acid (HEX) in solutions of distilled water were determined by using the DMA 4500 to determine their given densities for various molalities of each amino acid. The partial molal volume were determined to be $43.93 \pm 0.14 \ \frac{ml}{mol}$, $59.01 \pm 0.15 \frac{ml}{mol}$, $73.33 \pm 0.75 \frac{ml}{mol}$, and $93.81 \pm 0.44 \frac{ml}{mol}$ for glycine, β-alanine, GABA, and HEX respectively. Moreover, the apparent partial molal volumes were determined to be $41.87 \pm 0.16 \frac{ml}{mol}$, $58.33 \pm 0.31 \frac{ml}{mol}$, $70.49 \pm 1.10 \frac{ml}{mol}$, and $89.22 \pm 1.58 \frac{ml}{mol}$ for glycine, β-alanine, GABA, and HEX respectively.

INTRODUCTION

Density is defined as an intensive property, which characterises the solution. Density is also the mass per unit volume of the substance. Along with density, partial molal quantities are defined as the variation in properties, such as density, with respect to the number of moles of a substance that is added, with keeping all other variables constant. One partial molal quantity that can be easily measured is the partial molal volumes. Partial molal volumes are defined as the effective volume of a compound in a solution at infinite dilution and is determined by the intrinsic size of the molecule and the effects of the certain structure of the solvent on the surrounding molecules. The purpose of this experiment was to determine the partial molal volumes of four amino acids based on their respective calculated densities. Then, the average value for the methylene increment with the partial molar volume of each amino acid can be calculated and then further compared to values found online or in literature. The four amino acids that were analyzed were glycine, β-alanine, γ-aminobutyric acid (GABA), and 6-aminohexanoic acid (HEX).

PROCEDURE

Five different concentrations of glycine, β-alanine, GABA, and HEX were prepared in jars. The concentrations were ensured to be within the range of 0.01 to 0.1 molal. For each amino acid, the empty jar and its cap were weighed by using the analytical balance. After adding the amino acid into each jar, they were reweighed. About 20 mL of distilled water was added into each jar by using the graduated cylinder and the content was mixed well until all solutes dissolved. The jar and its cap were reweighed and all of these masses were recorded.

For each solution, their densities were measured by using the Anton Parr DMA 4500 Density Meter oscillating U-tube. The density measurements were made at 25.0 °C. For each amino acid, the density of distilled water was determined first. A disposable syringe was rinsed with distilled water and the solution was taken, and it was gently tapped to remove the air bubbles that might have formed. It was inserted into the machine at the injection port and about 3 mL of the solution were injected. The syringe was left in the machine until a measurement was obtained. The density was recorded after the word 'valid' appeared on the screen and reported to 0.XXXXX g/cm^3. A second trial was run to obtain a second density value. The measurements were ensured to agree within 0.0000X g/cm^3 or else another trial should be run. At least duplicate measurements of density were needed for each solution. The density of water obtained was compared with the known density at that temperature to ensure the instrument operated perfectly.

For the first amino acid, the density measurement was done with the same procedure as being done on distilled water, except only about 2 mL of the solution were injected. The density was recorded to 1.XXXXX g/cm^3 and the second density should agree by 0.0001 g/cm^3. These procedures were repeated for the other 4 different concentrations of glycine.

Before starting the density measurement of another amino acid, the syringe was rinsed with distilled water for three times and the machine was cleaned by injecting distilled water and pushing it through the port for three times. The water was removed by attaching the air hose into the waste container and the 'Pump' button was pressed. The button was pressed again to stop the pump. The entire procedures were repeated for a new set of amino acids, starting with the distilled water and the 5 solutions of amino acids.

The DM4500 CELL was rinsed with several portions of distilled water to remove the solutions to prevent contamination of the cell. The jars and caps were rinsed with distilled water and the jars, not the caps, were dried in the oven. All of the solutions were poured down the drain with running water.

RESULTS AND DISCUSSION

Table 1: Molality of each solution

Amino acid	Set #	W_1 (g)	W_2 (g)	W_3 (g)	W_A (g)	W_H (g)	Molality (m)
	1	88.6801	89.1798	108.4085	0.4997	19.2287	0.3462
	2	87.6229	87.8268	106.9540	0.2039	19.1272	0.1420
	3	88.3554	88.4289	107.0498	0.0735	18.6209	0.0526
	4	88.6995	89.6813	110.3386	0.9818	20.6573	0.6331
Glycine	5	87.0279	87.3346	107.2072	0.3067	19.8726	0.2056
	1	88.1254	88.5744	108.6049	0.4490	20.0305	0.2516
	2	88.9820	89.9004	109.7426	0.9184	19.8422	0.5195
	3	87.5225	88.3949	107.0590	0.8724	18.6641	0.5247
	4	89.5187	90.1919	110.2097	0.6732	20.0178	0.3775
β-alanine	5	88.3878	89.1935	108.6458	0.8057	19.4523	0.4649
	1	88.5268	88.8160	108.2424	0.2892	19.4264	0.1444
	2	88.5274	88.7803	107.6438	0.2529	18.8635	0.1300
	3	87.9989	88.2188	107.9849	0.2199	19.7661	0.1079
	4	88.3623	88.8299	109.0210	0.4676	20.1911	0.2246
GABA	5	88.7304	89.1504	108.9132	0.4200	19.7628	0.2061
	1	88.8626	88.9198	108.0126	0.0572	19.0928	0.0228
	2	88.6295	88.7958	107.9802	0.1663	19.1844	0.0661
	3	86.8786	87.0535	106.2906	0.1749	19.2371	0.0693
	4	88.8006	89.1597	108.8088	0.3591	19.6491	0.1393
HEX	5	88.4567	88.7433	108.1382	0.2866	19.3949	0.1127

W_1 - Weight of jar and cap
W_2 - Weight of jar, cap, and amino acids
W_3 - Weight of jar, cap, amino acids, and water
W_A - Weight of amino acids
W_H - Weight of water

Table 2: Molar mass of amino acids

Amino acid	Molar mass ($\frac{g}{mol}$)
Glycine	75.07
β-alanine	89.09
GABA	103.12
HEX	131.17

Table 1 shows the molality concentration for each solution of amino acids. Each set represents a different molality of amino acids solutions. In order to determine the molality, the weight of amino acids and distilled water in each jar were calculated by using Eq. 1 - 4 as listed below. The molar mass of each amino acid is as demonstrated in Table 2.

$$W_A\ (g) = W_2\ (g) - W_1\ (g) \quad \text{(Eq. 1)}$$

$$W_H\ (g) = W_3\ (g) - W_2\ (g) \quad \text{(Eq. 2)}$$

$$\text{Moles of amino acids (mol)} = W_A\ (g) \times \text{Molar mass } \left(\frac{g}{mol}\right) \quad \text{(Eq. 3)}$$

$$\text{Molality (m)} = \frac{moles\ of\ amino\ acids\ (mol)}{W_H\ (kg)} \quad \text{(Eq. 4)}$$

Table 3: Density measurements of each solution

Amino acids	Set #	Molality (m)	ρ_1 ($\frac{g}{cm^3}$)	ρ_2 ($\frac{g}{cm^3}$)	Agreement ($\frac{g}{cm^3}$)
Glycine	Pure	0.0000	0.99698	0.99696	0.00002
	1	0.3462	1.00779	1.00784	0.00005
	2	0.1420	1.00160	1.00158	0.00002
	3	0.0526	0.99873	0.99871	0.00002
	4	0.6331	1.01616	1.01629	0.00013
	5	0.2056	1.00354	1.00353	0.00001
β-alanine	Pure	0.0000	0.99707	0.99706	0.00001
	1	0.2516	1.00458	1.00459	0.00001
	2	0.5195	1.01217	1.01232	0.00015
	3	0.5247	1.01247	1.01247	0.00000
	4	0.3775	1.00840	1.00833	0.00007
	5	0.4649	1.01072	1.01078	0.00006

	Pure	0.0000	0.99693	0.99688	0.00005
	1	0.1444	1.00118	1.00128	0.00010
	2	0.1300	1.00079	1.00092	0.00013
	3	0.1079	1.00034	1.00033	0.00001
	4	0.2246	1.00363	1.00368	0.00005
GABA	5	0.2061	1.00271	1.00280	0.00009
	Pure	0.0000	0.99708	0.99707	0.00001
	1	0.0228	0.99808	0.99809	0.00001
	2	0.0661	0.99964	0.99967	0.00003
	3	0.0693	0.99965	0.99965	0.00000
	4	0.1393	1.00230	1.00234	0.00004
HEX	5	0.1127	1.00135	1.00134	0.00001

ρ_1 - density for first trial

ρ_2 - density for second trial

The density, ρ, of these solutions were as shown in Table 3. It was ensured that the measurements recorded for both trials agreed within 0.0001X $\frac{g}{cm^3}$. The pure set of solution for each amino acid was for the determination of density of distilled water.

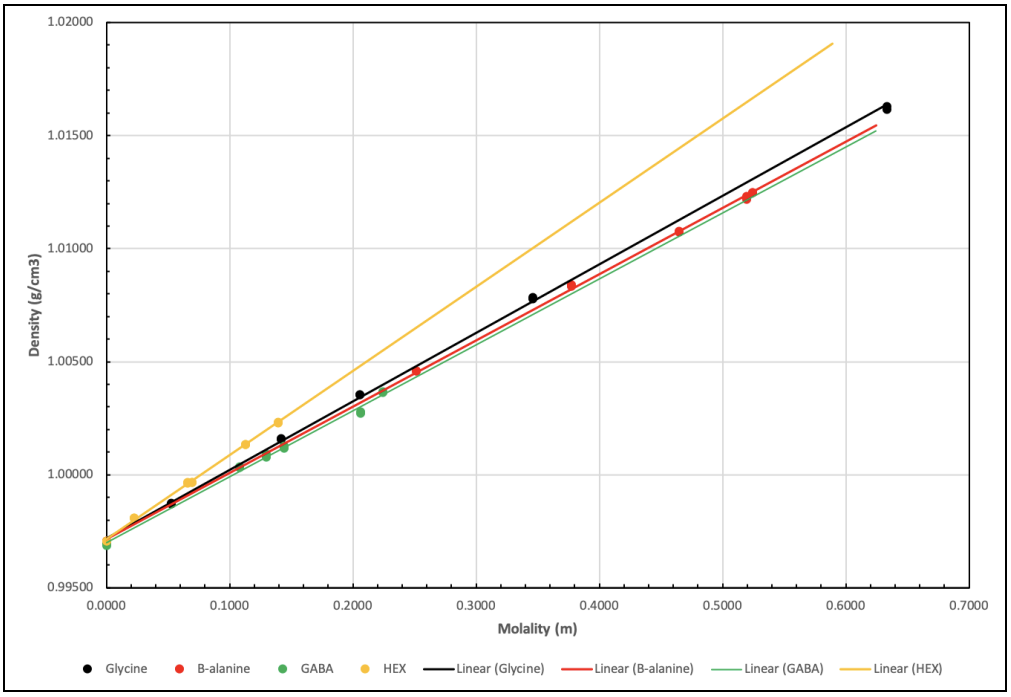

Figure 1: Graph of density versus molality for 4 different amino acids

The data points plotted in Figure 1 were each fitted with a linear trendline. As could be seen in that figure, most of the data points were higher than 0.1 m, which should not be the case since it should be ensured at the beginning of the experiment to have a range of molality concentration within 0.01 to 0.1 m. This happened due to experimental error in which the amount of amino acids added into the jars were overestimated and the expectation was that it still fell within the required range. The molality were not roughly calculated during the experiment, resulting in this bizarre dispersion of data points. In order to see the trend of each amino acid and to compare them with each other easily, the trendlines were extrapolated to a significant range. The equation for each trendline was as listed below:

Glycine: $\rho = 0.0303m + 0.9972$, $R^2 = 0.9995$

β-alanine: $\rho = 0.0293m + 0.9971$, $R^2 = 0.9997$

GABA: $\rho = 0.0291m + 0.9970$, $R^2 = 0.9951$

HEX: $\rho = 0.0372m + 0.9971$, $R^2 = 0.9988$

The slope represents how much the density changed as the molality changed at the same time. By looking at the slope and the trendline itself, it could be seen that HEX had higher density than glycine, which was higher than that of alanine and GABA, at least within the range of molality extrapolated for this experiment. As reflected by the value of R^2, the data points were perfectly fitted with a linear trendline, as the values of R^2 were close to 1, indicating how less likely the data points deviated from the trendline. However, the parameters of these trendlines have no fundamental significance.

Table 4: Volume of each solution

Amino acids	Set #	Molality (m)	V_1 (mL)	V_2 (mL)
	Pure	0.0000	1003.03	1003.05
	1	0.3462	1018.06	1018.01
	2	0.1420	1009.05	1009.07
	3	0.0526	1005.22	1005.24
	4	0.6331	1030.87	1030.74
Glycine	5	0.2056	1011.85	1011.86
	Pure	0.0000	1002.94	1002.95
	1	0.2516	1017.75	1017.74
	2	0.5195	1033.71	1033.55
	3	0.5247	1033.85	1033.85
	4	0.3775	1025.02	1025.09
β-alanine	5	0.4649	1030.37	1030.31
	Pure	0.0000	1003.08	1003.13
	1	0.1444	1013.69	1013.59
	2	0.1300	1012.61	1012.48
	3	0.1079	1010.78	1010.79
	4	0.2246	1019.46	1019.41
GABA	5	0.2061	1018.49	1018.40
	Pure	0.0000	1002.93	1002.94
	1	0.0228	1004.93	1004.92
	2	0.0661	1009.03	1009.00
	3	0.0693	1009.45	1009.45
	4	0.1393	1015.94	1015.90
HEX	5	0.1127	1013.41	1013.42

V_1 - volume for first trial
V_2 - volume for second trial

$$V\ (mL) = \frac{1000\ g\ of\ H_2O + [molality\ (\frac{mol}{kg}) \times 1\ kg \times molecular\ weight\ (\frac{g}{mol})]}{\rho\ of\ solution\ (\frac{g}{mL})},\ 1\ \frac{g}{mL} = 1\ \frac{g}{cm^3} \quad \text{(Eq. 5)}$$

The volume tabulated in Table 4 was calculated by using Eq. 5 as shown above. To calculate the volume of pure solution, the molality used was 0 m, since there were no amino acids added into the solution.

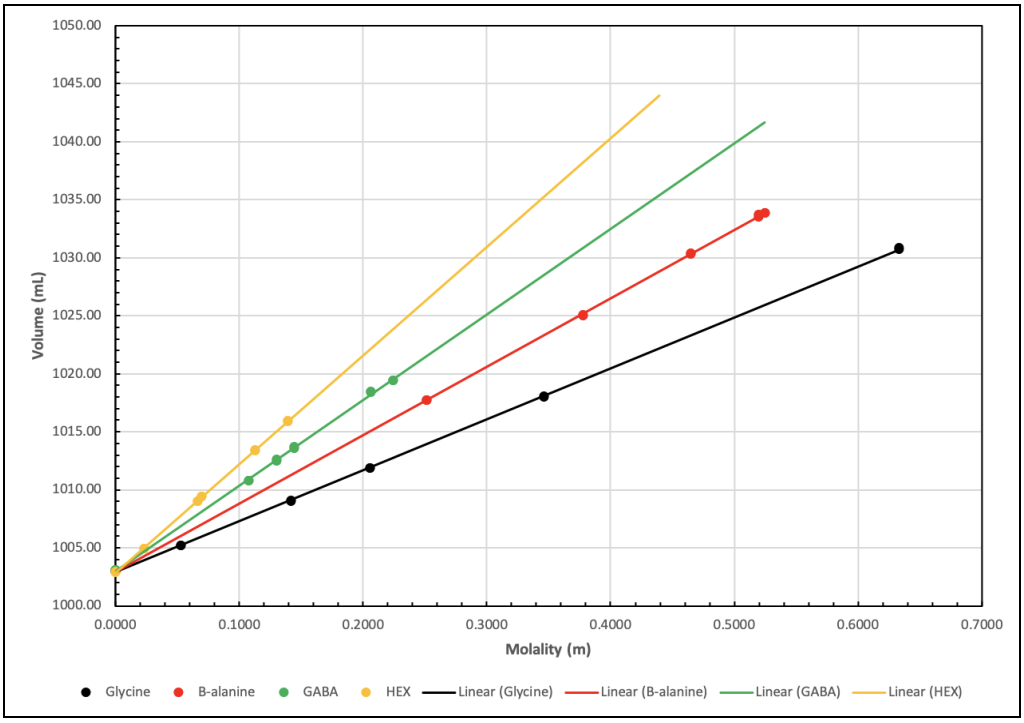

Figure 2: Graph of volume versus molality for 4 different amino acids

Illustrated in Figure 2 were data points that were fitted with a linear trendline for each set of amino acids. It could be seen that the trendline of HEX is steeper than that of GABA, along with that of alanine and glycine, from the steepest to the least steepest of trendline. The slope represented how much the volume of solution changed with respect to the molality change.

Table 4: Regression analysis of data points for Figure 2 for each amino acid

Amino acid	Slope ($\frac{mL}{m}$)	Uncertainty ($\frac{mL}{m}$)	Intercept (mL)	Uncertainty (mL)
Glycine	43.93	0.14	1002.903	0.043
β-alanine	59.01	0.15	1002.895	0.064
GABA	73.33	0.75	1003.02	0.12
HEX	93.81	0.44	1002.855	0.038

Regression analysis was performed on each of the data sets to determine the slope and intercept, with its respective uncertainty, as tabulated in Table 4 above. For a better representation of the trendline equations, they were as listed below:

Glycine: $V = (43.93 \pm 0.14)\ m + (1002.903 \pm 0.043)$

β-alanine: $V = (59.01 \pm 0.15)\ m + (1002.895 \pm 0.064)$

GABA: $V = (73.33 \pm 0.75)\ m + (1003.02 \pm 0.12)$

HEX: $V = (93.81 \pm 0.44)\ m + (1002.855 \pm 0.038)$

From these trendline equations, the partial molal volume of the amino acids, $\overline{V_2}$, in the solution could be determined by using Eq. 6 as shown below.

$\overline{V_2} = \left(\frac{\delta V}{\delta m}\right)_{T, P, n_1}$, where 1 is the solvent (water) and 2 is the amino acid (solute) (Eq. 6)

Table 5: Partial molal volume of amino acids

Amino acid	Volume ($\frac{ml}{mol}$)
Glycine	43.93
β-alanine	59.01
GABA	73.33
HEX	93.81

Since all of the trendlines were linear, Eq. 6 would result in constant value, $\overline{V_2}^0$, which was just the slope of the trendline. The values were as tabulated in Table 5 above. These partial molal volumes are the volumes at infinite dilution, where the amino acids interactions were no longer observed. Initially, since the unit of the slope is $\frac{ml}{m}$ **,** as the partial derivatives in Eq. 6 are the changes in volume per changes in molality, the partial molal volumes should have the same unit. However, partial molal volumes in general should have units of $\frac{ml}{mol}$ [1]. In order to generalize them, the partial derivatives were multiplied by mass of water (1 kg). This was the value used in Eq. 5. In this case, the values of partial molal volume would remain the same as the slope's.

Another model to determine the partial molal volume of amino acids in the solutions was by assuming the volume of solvent in the solution to be equivalent to the pure solvent's volume. The variation in the volume of solution was only affected by the amino acids. The volume of the amino acids in the solution was called apparent partial molal volume, Φ.

Table 6: Apparent partial molal volume of amino acids

Amino acids	Set #	Molality (m)	Φ_1 ($\frac{ml}{mol}$)	Φ_2 ($\frac{ml}{mol}$)
	1	0.3462	43.38	43.24
	2	0.1420	42.30	42.44
	3	0.0526	41.55	41.93
	4	0.6331	43.96	43.75
Glycine	5	0.2056	42.86	42.91
	1	0.2516	58.86	58.82
	2	0.5195	59.21	58.91
	3	0.5247	58.91	58.91
	4	0.3775	58.48	58.67
β-alanine	5	0.4649	59.00	58.87
	1	0.1444	73.33	72.63
	2	0.1300	73.09	72.08
	3	0.1079	71.16	71.25
	4	0.2246	72.82	72.59
GABA	5	0.2061	74.66	74.22
	1	0.0228	87.21	86.77
	2	0.0661	92.28	91.82
	3	0.0693	93.94	93.94
	4	0.1393	93.34	93.05
HEX	5	0.1127	92.99	93.08

Φ_1 - apparent partial molal volume for first trial
Φ_2 - apparent partial molal volume for second trial

$$\Phi\left(\frac{mL}{mol}\right) = \frac{MW}{\rho} - \frac{1000}{m} \times \left(\frac{\rho - \rho_0}{\rho \times \rho_0}\right); \text{(Eq. 7)}$$

MW - molecular weight of amino acids $\left(\frac{g}{mol}\right)$
m - molality of solution $\left(\frac{mol}{kg}\right)$
ρ - density of the solutions $\left(\frac{g}{mL}\right)$
ρ_0 - density of pure solvent $\left(\frac{g}{mL}\right)$

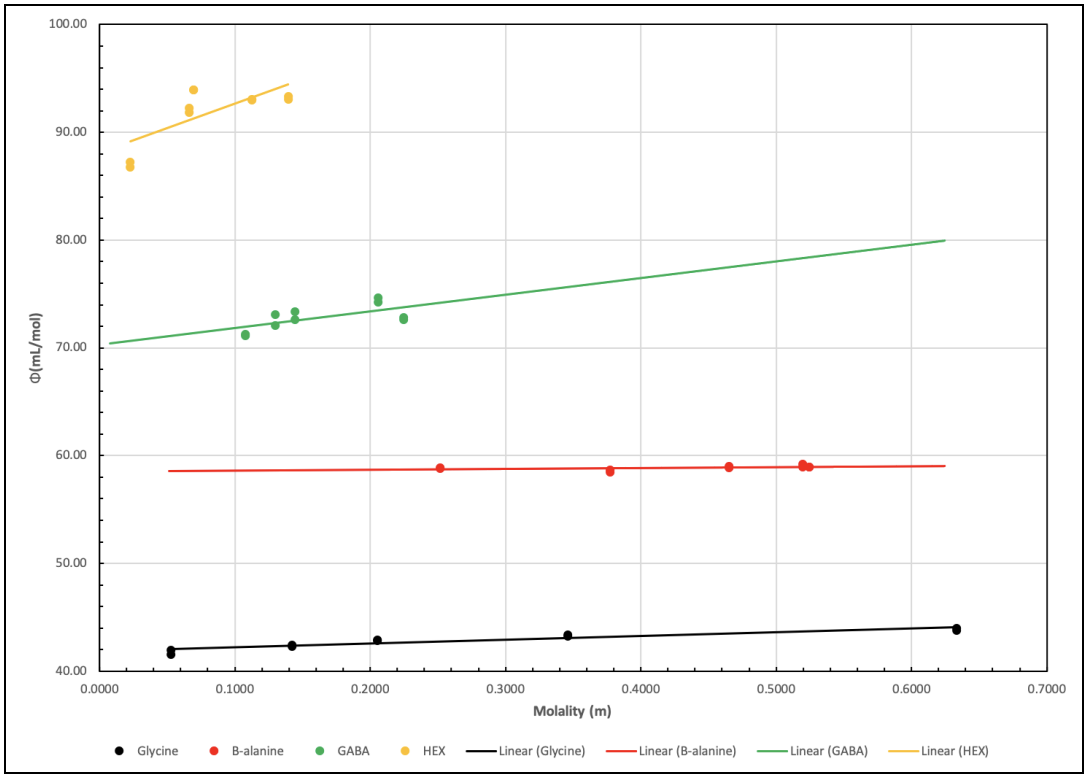

Figure 3: Graph of Φ versus molality for 4 different amino acids

By using Eq. 7, Φ was calculated and the values are as tabulated in Table 6. ρ_0 was determined by taking the average of the density of pure solvent from both trials as tabulated in Table 3 for each amino acid. By referring to Figure 3, the data points for each set were fitted with a linear trendline and were extrapolated with the same reason as mentioned earlier. In this figure, neither one of the data points were for pure solution, which was just distilled water. This was due to the assumption made by this model, where the volume of the solvent in the solution was exactly the volume of pure solvent, as previously mentioned. It did not make sense to have an 'apparent volume' of pure solvent since only the concentration of amino acids affected the volume of solution overall.

Table 7: Regression analysis of data points for Figure 3 for each amino acid

Amino acid	Slope ($\frac{mL}{mol \cdot m}$)	Uncertainty ($\frac{mL}{mol \cdot m}$)	Intercept ($\frac{mL}{mol}$)	Uncertainty($\frac{mL}{mol}$)
Glycine	3.35	0.46	41.87	0.16
β-alanine	1.21	0.67	58.33	0.31
GABA	12.2	6.5	70.49	1.10
HEX	35.4	16.5	89.22	1.58

Another set of regression analysis was performed on these data points to determine the slope and intercept, with their uncertainties, of the trendlines. The results were as tabulated in Table 7. The equations of trendlines could be written as shown below:

Glycine: $\Phi = (3.35 \pm 0.46)\ m + (41.87 \pm 0.16)$

β-alanine: $\Phi = (1.21 \pm 0.67)\ m + (58.33 \pm 0.31)$

GABA: $\Phi = (12.2 \pm 6.5)\ m + (70.49 \pm 1.10)$

HEX: $\Phi = (35.4 \pm 16.5)\ m + (89.22 \pm 1.58)$

Table 8: Partial molal volume from two different method

Amino acid	$\overline{V_2}^0$ ($\frac{mL}{mol}$)	Φ^0 ($\frac{mL}{mol}$)	**Differences** ($\frac{mL}{mol}$)
Glycine	43.93	41.87	2.06
β-alanine	59.01	58.33	0.68
GABA	73.33	70.49	2.84
HEX	93.81	89.22	4.59

The partial molal volume at infinite dilution could be obtained from two different methods; the derivative of volume as in Eq. 7 and from Figure 3. At infinite dilution, theoretically, $\Phi^0 = \overline{V_2}^0$. To find Φ^0, m is set to be equal to 0, which resulted in the value of intercept, and both Φ^0 and $\overline{V_2}^0$ were tabulated in Table 8. It could be seen that for all amino acids, these values did not agree with each other.

One of the main reasons causing these differences was due to the molality of solution prepared at the very beginning. It was noted that the determinations of densities at low concentration should be accurate, since they were only slightly different from the density of pure water. It was required to have as many as data points at lower molality, close to 0 m, in order to determine the partial molal volume at infinite dilution more precisely and accurately. As previously mentioned, due to experimental error, most of the solutions were prepared with molality of higher than 0.1 m. By comparing these two values for each amino acid, they did not deviate largely from each other (not by ~20-30 $\frac{mL}{mol}$), yet, it would still be considered as significant differences that could not be concluded to be in agreement with each other.

If this experiment were repeated to have a better data set, the solution should be prepared in a more precise manner. Since only about 20 mL of distilled water added into the jar, about $\frac{1}{16}$ or less of the spatula of amino acids should be added in the jar, in order to have molality within a range of 0.01m - 0.1m.

Table 9: Average partial molal volume of each amino acid

Amino Acid	Chemical Formula	x	$\overline{V_E}^0$ ($\frac{mL}{mol}$)
Glycine	$C_2H_5NO_2$	1	42.90
β-alanine	$C_3H_7NO_2$	2	58.67
GABA	$C_4H_9NO_2$	3	71.91
HEX	$C_6H_{13}NO_2$	5	91.52

The partial molal volumes of compounds in water depend primarily on the sizes of the compounds or ions, but are not directly proportional to them. In other words, it is related to the structural units in the molecule. It is examined that these amino acids have a common functional group, which is a methylene group ($-CH_2$), where x is denoted as the number of methylene groups in each amino acid. By using the data tabulated in Table 9, the average value for the methylene increment in the partial molal volumes of amino acids could be computed. The average partial molal volumes, $\overline{V_E}^0$ of each acid, were calculated by taking the average of partial molal volumes tabulated in Table 8 from both methods.

Table 10: Experimental and literature value [2] of partial molal volumes

Amino Acid	x	$\overline{V_E}^0$ ($\frac{mL}{mol}$)	$\overline{V_L}^0$ ($\frac{mL}{mol}$)	Differences ($\frac{mL}{mol}$)
Glycine	1	42.90	43.24	0.34
β-alanine	2	58.67	58.50	0.17
GABA	3	71.91	73.23	1.32
HEX	5	91.52	104.09	12.57

$\overline{V_E}^0$ - experimental partial molal volume

$\overline{V_L}^0$ - in-literature partial molal volume

Table 11: Regression analysis on data in Table 10

Type of data	Slope ($\frac{mL}{mol}$)	Uncertainty ($\frac{mL}{mol}$)	Intercept ($\frac{mL}{mol}$)	Uncertainty ($\frac{mL}{mol}$)
Experimental	14.51	0.73	28.8	1.6
Literature	15.00	0.15	28.33	0.33

Experimental: $\overline{V_E} = (14.51 \pm 0.72)\ x + (28.8 \pm 1.6)$ (Eq. 8)

Literature: $\overline{V_L} = (15.00 \pm 0.15)\ x + (28.33 \pm 0.33)$ (Eq. 9)

The literature values of partial molal volumes of each amino acid were tabulated and compared with the experimental value, as shown in Table 10. It could be seen from the differences that the values did not agree with each other. Due to this, it was expected that, after a regression analysis performed on these data, making x and $\overline{V_E}^0$ or $\overline{V_L}^0$ as the independent and dependent variable respectively, the partial molal volume change per increment of methylene group would be different. The results of the analysis were tabulated in Table 11.

The slope indicated the change in partial molal volume, as the number of methylene groups changed at the same time. It is found that the literature value had higher average methylene group increment in partial molal volume of these amino acids (except for HEX), where in the order of experimental and literature value, they were 14.51 $\frac{mL}{mol}$ and 15.00 $\frac{mL}{mol}$ **.** One of the main reasons that causes this different results was the different experimental skills exhibited by those who performed this experiment. Those people who obtained the literature values might have many experiences in the lab and were more thorough in their work. Moreover, the surrounding of the lab itself might be a factor making these large differences in the results obtained experimentally and from the literature.

Table 12: Prediction of partial molal volumes of each amino acid

Amino Acid	**x**	$\overline{V_E}^0$ ($\frac{mL}{mol}$)	$\overline{V_C}^0$ ($\frac{mL}{mol}$)	**Differences** ($\frac{mL}{mol}$)
Glycine	1	42.90	43.32	0.42
β-alanine	2	58.67	57.83	0.84
GABA	3	71.91	72.33	0.42
HEX	5	91.52	101.34	9.83

$\overline{V_E}^0$ - experimental partial molal volume

$\overline{V_C}^0$ - predicted/calculated partial molal volume

Eq. 8 was used to determine the partial molal volume of HEX, as tabulated in Table 12. It was observed that the differences in the first three acids were smaller than that of HEX. The results were expected because Eq. 8 was generated by using only the experimental data of the first three acids, but not of HEX's. Although the differences were small, they were still considered as significant differences, might be due to large uncertainties in the original data. By looking only at HEX, there was a large difference in partial molal volume between the experimental and calculated data. This was because, as mentioned previously, the solutions of each amino acid were not properly prepared. On top of that, Eq. 8 was obtained from data that already have large uncertainties, causing a domino effect, which heavily contributed to even larger uncertainty in these calculated data. The partial molal volume should be around the literature value tabulated in Table 10.

Table 13: Calculated partial molal volume from Solver function

Compound	x	$\overline{V_E}^0$ ($\frac{mL}{mol}$)	$\overline{V_C}^0$ ($\frac{mL}{mol}$)
CH_3COOH	0	51.9	51.3
CH_3CH_2COOH	1	67.9	67.4
$CH_3(CH_2)_2COOH$	2	84.6	83.6
$CH_3(CH_2)_3COOH$	3	100.5	99.7
$CH_3(CH_2)_4COOH$	4	116.0	115.9
HOOCCOOH	0	50.2	51.3
$HOOCCH_2COOH$	1	67.2	67.4
$HOOC(CH_2)_2COOH$	2	82.9	83.6
$HOOC(CH_2)_3COOH$	3	99.1	99.7
$HOOC(CH_2)_4COOH$	4	115.7	115.9
$HOOC(CH_2)_5COOH$	5	131.9	132.1

$\overline{V_E}^0$ - experimental/given partial molal volume

$\overline{V_C}^0$ - calculated partial molal volume

The amino acids used in this experiment were not sufficient to show the property of the structure with the partial molal volumes. A group contribution or quantitative structure-activity relationship (QSAR) [3] calculation was conducted on the given sets of partial molal volume of carboxylic acids, both mono- and di-carboxylic acids, as listed in Table 13. The calculated partial molal volume, $\overline{V_C}^0$, were obtained by using the Solver function in Excel.

Table 14: Regression analysis on data in Table 13

Slope ($\frac{mL}{mol}$)	Uncertainty ($\frac{mL}{mol}$)	Intercept ($\frac{mL}{mol}$)	Uncertainty ($\frac{mL}{mol}$)
16.16	0.13	51.26	0.37

To compare the average methylene group increment of the experimental data of amino acids with the given data of carboxylic acids, a regression analysis was again conducted on data values in Table 13, where x and $\overline{V_E}^0$ were the independent and dependent variables respectively. The results were tabulated in Table 14. Again, the slope indicated the average methylene group increment, which was 16.16 ± 0.13 $\frac{mL}{mol}$. In comparison with the results from the experimental data (14.51 ± 0.73 $\frac{mL}{mol}$ - Table 11), they did not agree with each other by 1.66 $\frac{mL}{mol}$. It should be the case considering the many flaws in conducting this experiment, as previously mentioned. The given data could be obtained by more professional scientists, which have more capability, knowledge and skills than what were possessed by the students.

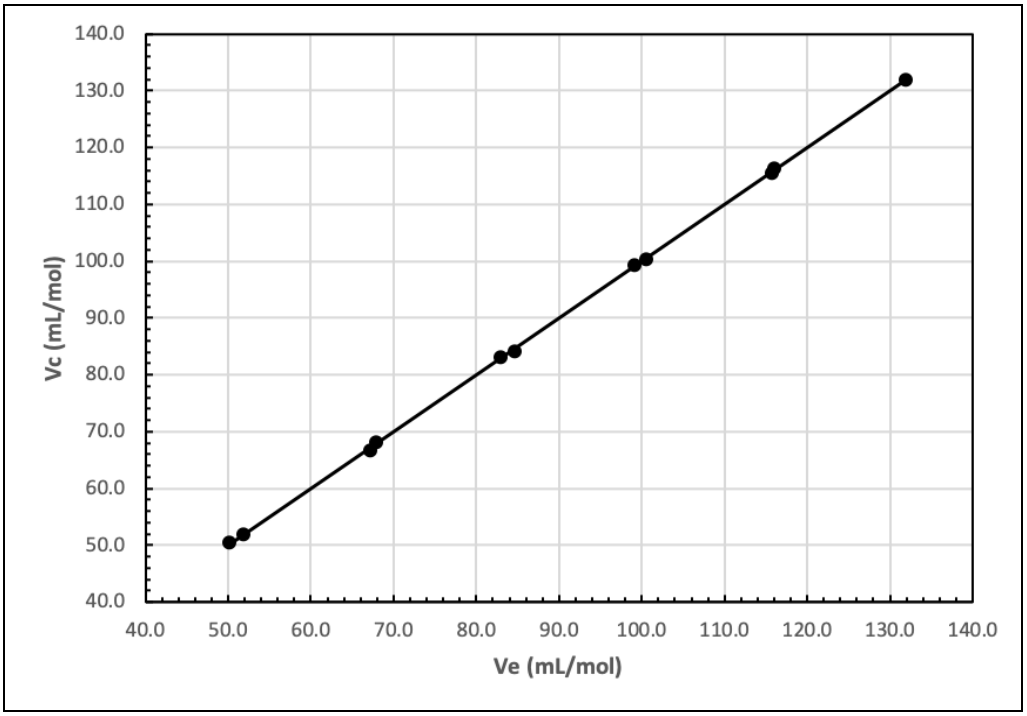

Figure 4: Graph of $\overline{V_C}^0$ versus $\overline{V_E}^0$ of the carboxylic acids

Table 15: Regression analysis on Figure 4

Slope	Uncertainty	Intercept ($\frac{mL}{mol}$)	Uncertainty ($\frac{mL}{mol}$)	R^2
0.9994	0.0081	0.05	0.75	0.9994

In order to determine whether $\overline{V_C}^0$ and $\overline{V_E}^0$ agree with each other more precisely, a regression analysis was conducted on the data sets used to plot Figure 4. The results of the analysis were tabulated in Table 15. The data points were fitted with a linear trendline and it could be seen that it could be fitted perfectly, by the value of R^2. The equation of the linear trendline could be written as shown below:

$$\overline{V_C}^0 = (0.9994 \pm 0.0081)\ \overline{V_E}^0 + (0.05 \pm 0.75) \quad \text{(Eq. 10)}$$

The slope of this plot indicated the change in $\overline{V_C}^0$ per changes in $\overline{V_E}^0$. The closer the value of slope is to 1, the higher the agreement between these two values of partial molal volume. For this plot, it was 0.9994 ± 0.0081, which could be said that it was fairly close to 1. It could be concluded that they were indeed in agreement with each other.

CONCLUSIONS

For four amino acids, the partial molal volume was determined with two different methods. Firstly, the densities of each amino acid were found using the DMA 4500 and then plotted against their respective molality of each solution, and from this, a linear relationship from both variables could be seen. Next, the volume was plotted against the molality of each solution and a linear trend line was fitted for each amino acid. From each trendline, the partial molal volume can be determined by taking the partial derivative, which is the first of two methods used in this experiment. The calculated partial molal volumes were $43.93 \pm 0.14 \ \frac{ml}{mol}$, $59.01 \pm 0.15 \frac{ml}{mol}$, $73.33 \pm 0.75 \frac{ml}{mol}$, and $93.81 \pm 0.44 \frac{ml}{mol}$ for glycine, β-alanine, GABA and HEX respectively. Meanwhile, the apparent partial molal volumes were calculated using the second method, which were determined, in the order of glycine, β-alanine, GABA, and HEX, to be $41.87 \pm 0.16 \frac{ml}{mol}$, $58.33 \pm 0.31 \frac{ml}{mol}$, $70.49 \pm 1.10 \frac{ml}{mol}$, and $89.22 \pm 1.58 \frac{ml}{mol}$. When comparing the partial molal volumes with their respective apparent partial molal volumes, the differences are 2.06 $\frac{ml}{mol}$, 0.68 $\frac{ml}{mol}$, 2.84 $\frac{ml}{mol}$, and 4.59 $\frac{ml}{mol}$, for glycine, β-alanine, GABA, and HEX respectively. Moreover, when comparing the experimental partial molal volumes with their respective apparent partial molal volumes found in literature, the differences are 0.34 $\frac{ml}{mol}$, 0.17 $\frac{ml}{mol}$, 1.32 $\frac{ml}{mol}$, and 12.57 $\frac{ml}{mol}$, for glycine, β-alanine, GABA, and HEX respectively.

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