NTU Journal of Pure Sciences (2025) 4 (2) : 9 - 21
DOI: https://doi.org/10.56286/ntujps.v1i3

IRAQI Academic Scientific Journals

ISSN: 2789-1089 EISSN: 2789-1097
NTU Journal of Pure Sciences
Available online at: https://journals.ntu.edu.iq/index.php/NTU-JPS/index

Thermodynamic study of pantothenic acid in different solvents and temperatures: Treatment by theoretical study

1st Khalil B.Rasho*1 , 2nd Fanar M. Al-Healy1
[1,2]Department of Chemistry, College of Sciences, University of Mosul, Mosul, Iraq
*Corresponding author E-mail: Khalil93barakat@gmail.com

Article Informations

Received: 17-07- 2024
Accepted: 19-05-2025
Published online: 30-06-2025

Corresponding author:
Name: Khalil B.Rasho
Affiliation : [1]Department of Chemistry, College of Sciences, University of Mosul, Mosul, Iraq
Email:Khalil93barakat@gmail.com

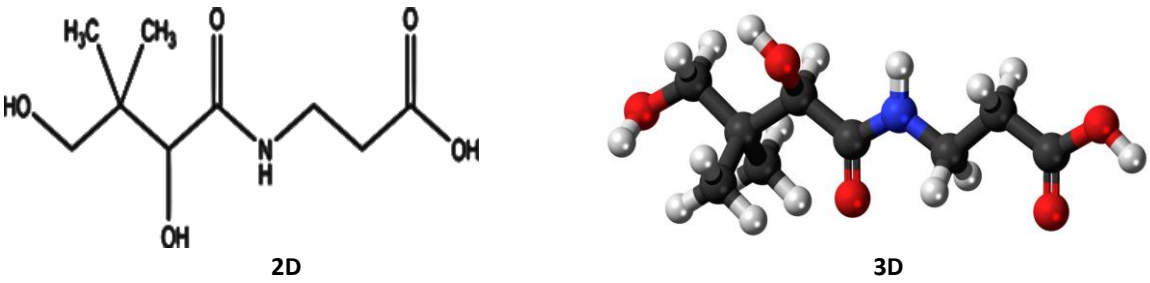
Key Words:
Electrical Conductivity, Pantothenic Acid, Theoretical Chemistry, Lee-Wheaton equation, DFT.

A B S T R A C T

Vitamin B5 (pantothenic acid) was studied thermodynamically by calculating its conductivity parameters, like association constant Ka, equivalent conductance at infinite dilution Λ_o, ionic conductivity, and the main distance between ions in solution (R) at best-fit values of (ϭΛ). The values of Ka, Λ_o, and R were measured for equivalent conductivities in different solvents — water and methanol — at varying temperatures between 293 K and 313 K, as well as in mixtures of methanol and water containing 10%, 20%, 30%, 40%, and 50% methanol at 310 K. The experimental data were treated by the Lee-Wheaton conductivity equation of symmetrical electrolytes (1:1) and were found be different from one solvent to another depending on the molecular interactions in the solution. Also, their physical parameters (viscosity & Dielectric constant) for each solvent were measured. Finally, thermodynamic quantities for the ion association reaction (ΔG, ΔH and ΔS) have been studied. Density functional theory DFT calculations, (B3LYP/6-31g(d,p)) were employed to analyze vitamin B5 in the gas phase and diverse solvents. Three different continuity methods, namely AM1, PM3, and HF, were utilized, followed by DFT. The final method was applied to explore the effects on its characteristics.

Introduction

Vitamin B5, or pantothenic acid, is one of the B-complex vitamins. Like the other water-soluble vitamins (B and C), it cannot be stored by the body. For this reason, we need to obtain it regularly. It has a specific chemical structure.



Scheme of 2D, & 3D structure of pantothenic acid

American biochemist Roger J. Williams isolated pantothenic acid as a growth factor in 1931[2]. Due to its great importance in the metabolism process, any deficiencyof vitamin B5 can lead to many health problems including metabolic disorders. pantothenic acid is a small molecule present in the living system, where it does several physiological functions. It is an essential nutrient to human health present in coenzyme A (CoA), an essential molecule in many key metabolic pathways [3]. Pantothenic acid is also found in acyl-carrier protein (ACP), which plays an important role in the biological synthesis of fatty acids. Although it is derived from the bacterial cell, it is the same and does not differ whether it is found in plants, animals, bacteria, or yeast. Syndrome forms of CoA deficiency due to a multitude of genetic mutations are becoming more frequent and cause cardiovascular diseases. CoA participates in the catabolism of amino acids with the formation of propionic and acetyl derivatives, which enter the cycle of the citric acid to provide energy. [4,5]

Electrochemistry is a branch of chemistry that deals with the study of the conversion between electrical and chemical energy which results from the movement of electrons or ions in chemical systems, which leads to the generation of electrical energy or the use of electrical energy to drive non-spontaneous chemical reactions. Electrochemistry is an interdisciplinary field that combines aspects of physics, chemistry, and engineering to study the interplay between electricity and chemical reactions. Electrical conductivity is the property that shows the ability of a material to conduct electrical current, or it is a measurement of the transfer of electrons or electrical charge by the material [6].

In this study, conductivity was measured using the Kohlrausch equation, and after obtaining the data, it was processed using the (L-W) equation to calculate thermodynamic values (ΔG, ΔH, and ΔS).

As thermodynamic parameters were calculated practically (by measuring the conductivity of the material), they were also calculated theoretically (quantum chemistry by using the DFT/B3LYP method at the 6-31G (d, p) basis set). These computations included HOMO-LUMO studies and molecular geometry structure optimization [7] as the calculations were made using density function theory (DFT), which is considered a compromise between calculation time, accuracy and quality of results compared to other methods that speed depends in calculation instead of accuracy and quality. DFT calculations provide good levels of accuracy compared to the computational

time, and are less expensive in terms of computational resources compared to other approaches used in addition to avoiding the wave function and using electron density instead [8].

EXPERIMENTAL:

Conductivity measurement:

The electrical conductivity of (pantothenic acid) was measured in a different solvent, which is water, methanol, and a mixture of methanol and water in different proportions (10%, 20%, 30%, 40%, 50%) and at different temperatures (20, 25, 30, 35, 40) ˚C but the mixture was measured at 37˚C using a WTW Inolab (740) Therminal740, (2003) computerized conductivity meter (made in Germany) [9]. A 0.000219 g of pantothenic acid (manufactured by BDH) was used as stock solution and prepared using Sartoins (5dis) (1995) MP, and dissolved in 10 ml of each solvent. A plastic syringe (1 ml) was used to inject a specific, balanced amount of the stock solution into the conduction cell and placed in a water bath to stabilize the temperature at the required degree. The cell was weighed before and after each addition of the solution to the cell, and the conductivity was determined after the additions.

Quantum Chemical Computations:

The Chemistry program, Chem 3DChemOffice software version 16.0 (level: Ultra) was used to perform theoretical calculations on the molecule by applying semi-empirical methods (AM1, PM3, HF). Finally, calculations were made based on the density functional theory DFT at B3LYP level with a 6-31G (d, p), by the final method the energy minimization of the molecule was performed the energy values of HOMO and LUMO were calculated after reaching the lowest energy level for the molecule, and through these values, many theoretical descriptions of the molecule are obtained [10].

RESULTS & DISCUSSION:

In conductivity measurements (pantothenic acid), the equation of Kohlrausch was used to detect types of pantothenic acid electrolytes by plotting the relation between equivalent conductivity against the square root of concentration at different solvents and temperature. The special calculation program was used to find the equivalent conductivity when entering the conductivity result and parameter, at different temperatures. and weights of the additives [11]. The positive ion is M^+ and negative ion is X^-. The equation for these solutions can be explained as follows.

$$MX_{aq} \overset{K_a}{\rightarrow} M^{+}_{aq} + X^{-}_{aq}$$

Ka: association constant

This relation has established that the solution is weak electrolyte behavior when the electrical conductivity was measured at different temperatures of the solution and all solvents. It is of the symmetrical electrolytes of (1:1) type. The tables and figures (1) (A-B-C) show the (pantothenic acid) behavior.

Table (1A). Equivalent conductivities (Λ) of (pantothenic acid) as a function of √Conc. at (293 to 313) K in water

Conc. (mole/L) * 10^{-6}	$\sqrt{C}$ (mole/L) $*10^{-4}$	Λ $\Omega^{-1}.equive^{-1}.cm$ 293 K	Λ $\Omega^{-1}.equive^{-1}.cm$ 298 K	Λ $\Omega^{-1}.equive^{-1}.cn$ 303 K	Λ $\Omega^{-1}.equive^{-1}.cm$ 308 K	Λ $\Omega^{-1}.equive^{-1}.cn$ 313 K
0.50	7.1061	198.0302	243.3675	246.5407	270.2717	313.8221
1.04	10.2048	120.0315	178.6396	182.6620	185.5579	189.2898
1.55	12.4459	112.9742	155.6370	157.4032	158.9473	178.0914
1.99	14.1130	100.4130	142.7707	143.8303	144.5439	156.8315
2.47	15.7112	101.2786	142.5758	125.8977	137.7185	157.8512
2.96	17.2003	101.4022	138.5938	114.9746	132.3436	148.3903
3.40	18.4422	102.9056	126.8827	113.4138	128.7459	142.5619
3.89	19.7165	102.8960	123.9329	112.9121	125.2047	136.7311
4.29	20.7201	98.9932	117.8300	106.8411	124.1530	134.7175
4.76	21.8192	99.7737	111.4179	106.1176	122.8687	131.7736
5.30	23.0170	99.0968	113.3716	105.5263	121.2686	127.7975
5.73	23.9466	100.2720	113.5250	106.0822	120.1891	126.6922
6.19	24.8798	100.9678	113.3356	106.8149	120.6257	122.0643
6.66	25.8119	100.9678	110.4010	110.5433	121.5480	118.6447

Fig (1A). Equivalent conductivities (Λ) of (pantothenic acid) as a function of √Conc. at (293 to 313)K in water

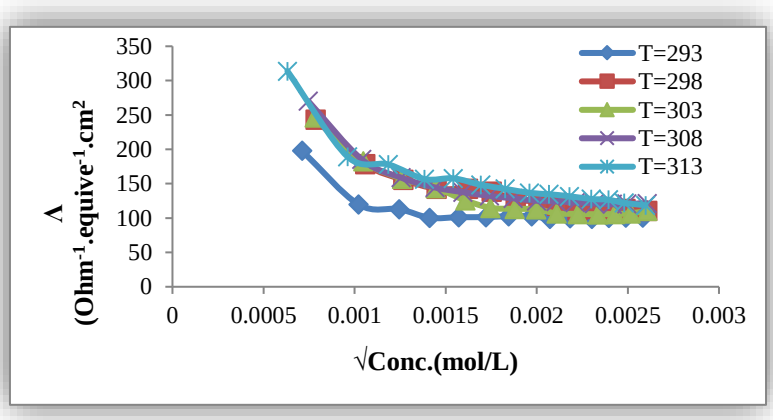
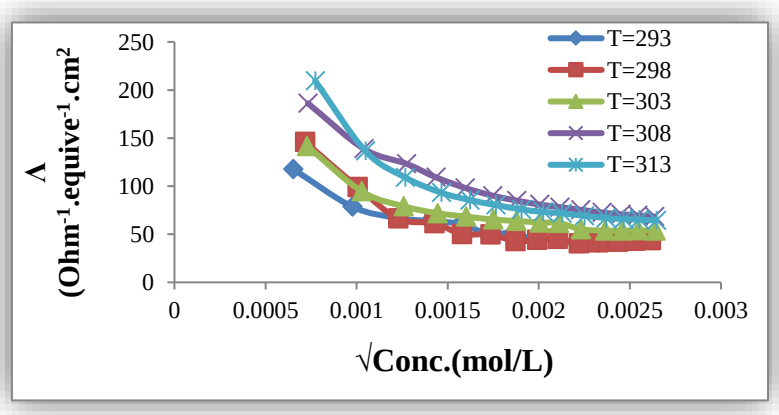


Table (1B): Equivalent conductivities (Λ) of (pantothenic acid) as a function of √Conc. at (293 to 313) K in methanol

Conc. (mole/L) *10^{-6}	$\sqrt{C}$ (mole/L)* 10^{-4}	Λ $\Omega^{-1}.equive^{-1}.cm$ 293 K	Λ $\Omega^{-1}.equive^{-1}.cm$ 298 K	Λ $\Omega^{-1}.equive^{-1}.cm^2$ 303 K	Λ $\Omega^{-1}.equive^{-1}.cm^2$ 308K	Λ $\Omega^{-1}.equive^{-1}.cm^2$ 313 K
0.42	6.51689	117.7307	146.0928	141.7121	186.0647	209.5256
0.95	9.76126	78.71349	99.02074	94.60233	138.835	136.5417
1.49	12.2179	66.98885	66.2931	79.10204	123.2813	109.0506
1.96	13.9991	63.78373	61.48945	71.85432	109.2555	93.26701
2.46	15.7001	60.85318	50.20188	68.30558	98.14953	85.5228
2.94	17.1442	51.03344	49.89357	65.32301	90.08762	80.42044
3.44	18.5482	50.86657	42.87634	63.87558	85.00153	75.82999
3.93	19.8331	44.48916	44.13743	62.2141	80.92036	73.24194
4.38	20.9239	45.68164	45.22192	61.75172	78.1858	71.84298
4.87	22.0746	41.04329	40.61666	55.2084	75.46986	69.13338
5.43	23.3032	41.43349	41.55581	53.71219	72.59599	66.90057
5.92	24.3299	42.23357	42.18422	53.77672	70.7514	65.82214
6.38	25.2543	43.11824	43.03019	53.99051	69.63491	65.26734
6.87	26.2033	43.69272	43.86743	53.79629	68.39578	64.31647

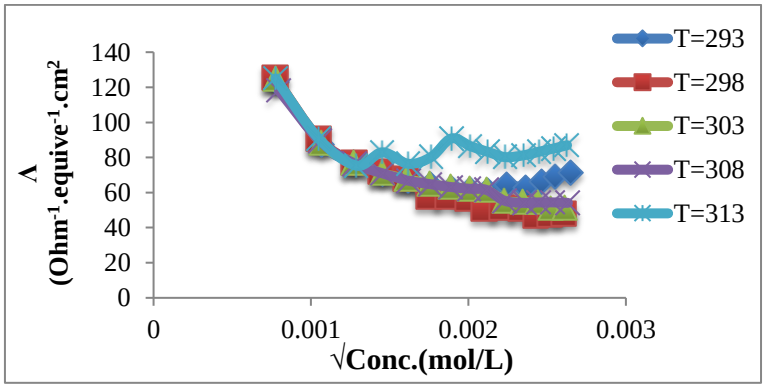


Fig(1B): Equivalent conductivities (Λ) of (pantothenic acid) as a function of √Conc. at (293 to 313) K in methanol

Table (1C): Equivalent conductivities (Λ) of (pantothenic acid) as a function of √Conc. at (310 K) in different percentages

Con. (mole/ L)*10^{-6}	$\sqrt{C}$ (mole/L) *10^{-4}	Λ $\Omega^{-1}.equive^{-1}.cm$ 10%	Λ $\Omega^{-1}.equive^{-1}.cm$ 20%	Λ $\Omega^{-1}.equive^{-1}.cm$ 30%	Λ $\Omega^{-1}.equive^{-1}.cm$ 40%	Λ $\Omega^{-1}.equive^{-1}.cm$ 50%
0.61	7.81233	122.8851	125.3548	124.6659	118.1304	125.0718
1.15	10.7132	87.1277	90.75523	88.30489	89.30673	90.69615
1.62	12.7281	77.15809	76.7934	77.09484	76.37305	75.33933
2.12	14.5491	70.86243	71.59707	71.02586	70.97057	82.91734
2.61	16.1684	66.9426	67.9775	67.81193	66.74497	76.37881
3.10	17.6189	64.42744	57.3663	64.94022	64.78965	80.32446
3.60	18.9630	62.56976	57.38685	63.22559	63.1604	90.83236
4.05	20.1197	61.75835	56.52405	61.98586	62.18026	86.43451
4.50	21.2151	61.0998	50.93393	61.40456	61.4964	83.21629
5.04	22.4591	64.43137	50.9827	55.42263	55.31709	80.20132
5.59	23.6370	62.6442	50.56117	54.5904	54.12041	81.27934
6.06	24.6265	65.95596	46.61668	54.57127	54.37566	83.30844
6.51	25.5064	69.16913	47.24799	51.02251	54.38648	85.13213
7.03	26.5048	71.17393	47.77404	51.27103	54.13757	86.98257

of the mixture



Fig(1D): Equivalent conductivities (Λ) of **(pantothenic acid)** as a function of √Conc. at (310 K) in different percentages of the mixture.

By using different solvents and at different temperatures, it is noticed that when increasing the temperature, the conductivity value increased. This indicates when an increase in temperature ions gain more energy thus increasing the ability to transfer electricity and conductivity [12]. In addition, the dielectric constant of solvents affects the conductivity value. Whenever the number of free ions increased, the electrical conductivity increased [13]. The(L-W) equation was used to calculate the equivalent conductivities at infinite dilution (Λ_o), association constant (Ka), the distance between ion R (A°), and stander deviation σΛ of the (pantothenic acid) solution described above, the special program was used to analyzed using a special analysis software after giving him information about the measurements, such as fixed cell concentrations (0.5cm), concentration, equivalent conductivity values and (density, a viscosity of the solution and dielectric constant) depend on changes in temperature and solvent. Table (2) shows values of Ka, Λ, R, and σΛ of (pantothenic acid).

Table 2: The values of Ka, Λ, R and σΛ of (pantothenic acid) at different (temperatures & solvents) .

		Water		
T (K)	Ka	Λ_o	R (Å)	δΛ
293	206560	160.101	1	0.14
298	877028	304.373	1	0.08
303	1424414	344.202	1	0.09
308	787381	304.942	1	0.13
313	1077300	357.761	1	0.14
		Methanol		
T(K)	Ka	Λ_o	R (Å)	δΛ
293	1966386	187.446	1	0.03
298	2846185	199.948	1	0.10
303	2714991	205.522	1	0.05
308	4025207	375.395	1	0.02
313	5278404	409.294	1	0.09
		Mixture		
%	Ka	Λ_o	R (Å)	δΛ
10%	183411	103.699	1	0.08
20%	3890887	248.655	1	0.02
30%	1215781	167.546	1	0.04
40%	854667	148.291	1	0.03
50%	30620	95.314	1	0.09

The results show that a cation is associated with an anion to form a Contact Ion–Pair (CIP) and was formed because the distance between the cation and anion is less than 2(Å). The values of σΛ are very small indicating that this equation was suitable for this study.

Thermodynamic study

The Vant-Hoff equation was used to calculate the thermodynamic parameters [14]. The values of ΔH were calculated from the slope the ΔG and ΔS values were calculated from:

This relationship gave a straight line of pyridoxine solutions,

$$LnKa = -\frac{\Delta H}{RT} + C \quad \ldots\ldots\ldots(1)$$

$$\Delta G = -RTLnKa$$

$$\Delta G = \Delta H\text{-}T\,\Delta S$$

Table 3B. Thermodynamic parameters of (pantothenic acid)

Water

T (K)	(1/T) (K^{-1})	ΔS ($J.mol^{-1}.K^{-1}$)	ΔG ($KJ.mol^{-1}$)	ΔH ($KJ.mol^{-1}$)	LnKa
293	0.003413	269.47	-29.79	49.16	12.23
298	0.003356	278.71	-33.89		13.68
303	0.003300	280.06	-35.69		14.17
308	0.003247	272.44	-34.74		13.57
313	0.003195	272.47	-36.11		13.88

Methanol

T (K)	(1/T) (K^{-1})	ΔS ($J.mol^{-1}.K^{-1}$)	ΔG ($KJ.mol^{-1}$)	ΔH ($KJ.mol^{-1}$)	LnKa
293	0.003413	241.05	-35.29	35.33	14.49
298	0.003356	242.11	-36.81		14.86
303	0.003300	239.74	-37.30		14.81
308	0.003247	241.08	-38.92		15.20
313	0.003195	241.50	-40.25		15.47

From the result we note the values of ΔH in water (enthalpy of association) were positive the dissociation is endothermic in water and negative in methanol, due to dielectric constant of water is greater than the dielectric constant of methanol. We also note that the values of ΔS were also positive due to the increase in randomness with increasing temperature, while ΔG (Gibbs free energy) has a negative value which means that the reaction was spontaneous towards association, and the due to the positive values of ΔH which leads to the ordering of the system as a result of association under the influence of solvation and columbic effect in spontaneous continuum media [15].

By plotting the relation between $\ln k_a \ against \ \frac{1}{T}$ was shown in Figure (2 , 3). This relationship gave a straight line of pyridoxine solutions

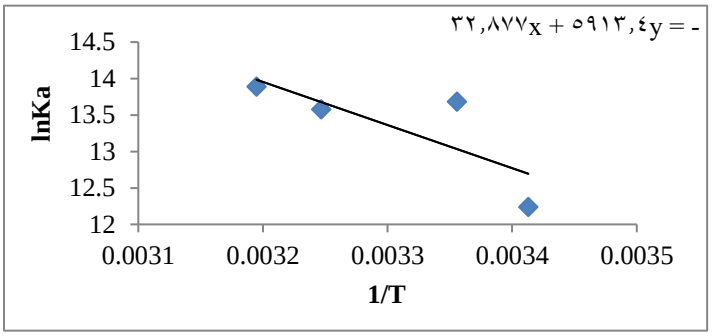


Fig (2) : The relation between ln k_a $against$ $\frac{1}{T}$ of $(pantothenic\ acid)$ in water

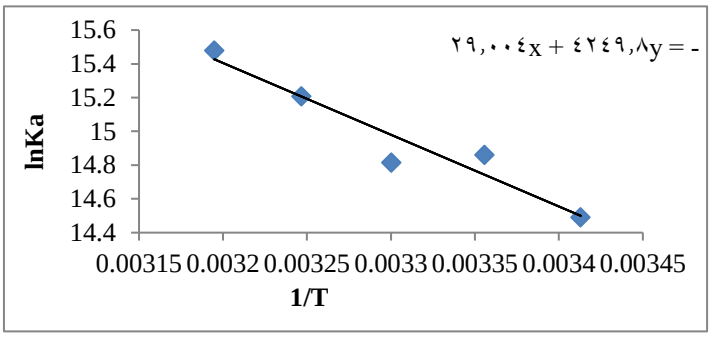


Fig (3) : The relation between ln k_a $against$ $\frac{1}{T}$ of $(pantothenic\ acid)$ in methanol

Walden Product

We used the Walden equation to calculate The walden product (Λoη) for studied (pantothenic acid).

$$\eta\ \Lambda^{\circ} = constant$$

The mixture of methanol in water was obtained by multiplying each value of (Λo) from Table (2) by viscosity (η) in (310 K) [16]. We can show the effect of viscosity and decently at different percentages. All results are listed in Table 4.

Table 4: Walden product against percentage of methanol in water at (310 K)

Percentage %	η	Λo	ηΛ
10%	0.00109	103.699	0.113
20%	0.00150	248.655	0.373
30%	0.00190	167.546	0.318
40%	0.00231	148.291	0.342
50%	0.00271	95.314	0.258

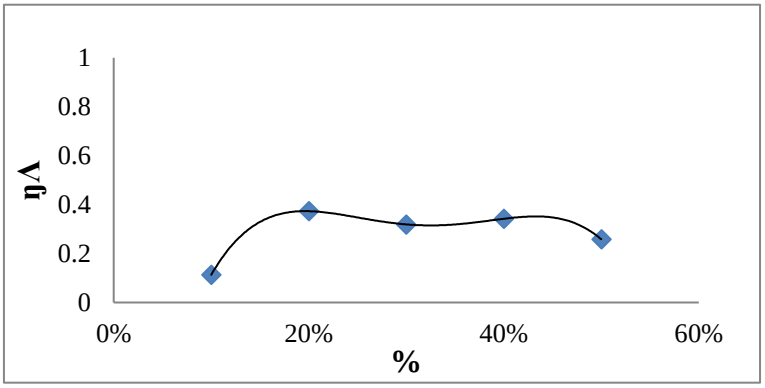


Fig (4): The relation between Walden product against percentage of methanol in water at (310 K)

Theoretical discussion:

Conceptual Density Functional Theory (DFT) or Chemical Reactivity Theory (as it is also known) is a powerful tool for predicting, analyzing, and interpreting the outcomes of chemical interactions. In this study, a series of molecular descriptors and attributes of their optimal geometries were calculated using density functional theory (DFT) and thermodynamics modeling [17].(Dehdab et al, 2016). The minimum energy was determined by various approaches of theoretical indexed in table 5.

Table 5: The energy values of each approach used in theoretical calculation.

	GAS PHASE				WATER	METHANOL
	AM1	PM3	HF	DFT	DFT	DFT
Finished energy Kcal/mol	-246.58	-241.51	-488919.15	-491865.46	-491882.03	-491881.67
ƐHOMO	-0.42254	-0.42179	-0.45826	-0.28877	-0.29305	-0.29618
ƐLUMO	0.03070	0.02665	0.13805	-0.01249	-0.01387	-0.01319

Physico-chemical descriptors play a crucial role in comprehending the reactivity of a molecule or system, and they are determined by analyzing the energy levels of the HOMO and LUMO. According to literature, the HOMO tends to donate electron density, whereas the LUMO acts as an electron acceptor. The energy gap between the HOMO and LUMO, known as EL-H, is utilized to elucidate the reactivity of the molecules under investigation. When water is used as a solvent, even a slight alteration in stability becomes apparent. Chemical hardness and softness (S) are employed to assess the reactivity and stability of the molecule or system. It has been noted that a higher softness or lower hardness value signifies increased polarization within the molecule or system. All descriptors determined from DFT energies can be listed in Table (6) [18].

Table (6): Descriptors calculated from DFT –HOMO, and LUMO energies.

Systems / Descriptors	GAS	WATER	METHANOL
HOMO (eV)	-0.28877	-0.29305	-0.29618
LUMO (eV)	-0.01249	-0.01387	-0.01319
GAP (ΔEL-H) (eV)	0.27628	0.27918	0.28299
Ionization potential (I)	0.28877	0.29305	0.29618
Electronic affinity (A)	0.01249	0.01387	0.01319
Hardness	0.13814	0.13959	0.141495
Softness	3.61951	3.58191	3.53369
Chemical potential (μ)	-0.15063	-0.15346	-0.154685
Electrophilicity (ω)	0.08212466	0.08435407	0.08455228

After completing the theoretical minimizing, some properties of the molecule (B5) in gas, water, and methanol Solvent as shown in Table (7)were computed. From the values of these descriptors, we can see the solvent effect on them like Connolly parameters which decreased in the solvents than the gas system. Also, the molecular volume is one of the important descriptors that varies when the system changes, its value was (1723.481, 1711.815, and 1712.033) in gas, water, and methanol systems respectively. The big value is in gas because there is no effect on the molecule, while it will be decreased in water and more in methanol so the methanol system is more affected by the molecular volume. This can be reflected in the equivalent conductivity values upon infinite dilution at a temperature of 298 K (Λ_o), as we notice that the value in water is higher than in methanol, (Λ_o) in water at 298K = Λ_o = 248.285 $S \cdot cm^2 \cdot mol^{-1}$in methanol at 298K = 87.158 $S.eq^{-1}.cm^2$.

Table (7): DFT descriptors of the B5 molecule in three systems

Descriptors	Gas	WATER	METHANOL
Lipinski Rule	219.111; 4; 4; 7; -1.494	219.111; 4; 4; 7; -1.494	219.111; 4; 4; 7; -1.494
Connolly Accessible Area (A°2)	357.024 Angstroms Squared	356.731 Angstroms Squared	356.739 Angstroms Squared
Connolly Molecular Area (A°2)	175.349 Angstroms Squared	175.382 Angstroms Squared	175.385 Angstroms Squared
Connolly Solvent Excluded Volume (A°3)	145.469 Angstroms Cubed	145.527 Angstroms Cubed	145.53 Angstroms Cubed
Number of H Bond Acceptors	4	4	4
Number of H Bond Donors	4	4	4
Dipole (Debye)	6.9829 Debye	7.2446 Debye	7.2341 Debye
Molecular Volume (bohr^3/mol	1530.778 bohr**3/mol	1974.412 bohr**3/mol	1888.869 bohr**3/mol
RMS Force (Kcal/mol)	6.7283 Kcal/Mol	8.0195 Kcal/Mol	7.9771 Kcal/Mol
SCF Energy (Kcal/mol)	-488912.69 Kcal/Mol	-488910.17 Kcal/Mol	-488910.25 Kcal/Mol
Entropy (Cal/mol-Kelvin)	112.29 Cal/Mol-Kelvin	112.232 Cal/Mol-Kelvin	112.235 Cal/Mol-Kelvin
Molecular Mass (au)	219.11067 au.	219.11067 au.	219.11067 au.
Thermodynamic Energy (Kcal/mol)	190.35 Kcal/Mol	190.15 Kcal/Mol	190.155 Kcal/Mol
Zero-Point Energy (Kcal/mol)	181.898531 Kcal/Mol	181.718436 Kcal/Mol	181.723456 Kcal/Mol

Descriptors	Gas	WATER	METHANOL
Polarizability	135.6148 2.2622 102.7741 2.2621 1.3992 82.7161	135.4838 3.0902 103.047 3.1385 1.5727 83.0964	135.483 3.0734 103.0424 3.1198 1.5713 83.0848
	Molecular Topology Descriptors		
Balaban Index	172022	172022	172022
Cluster Count	15	15	15
Molecular Topological Index	2718	2718	2718
Num Rotatable Bonds	7 Bond(s)	7 Bond(s)	7 Bond(s)
Polar Surface Area (A°2)	106.86 Angstroms Squared	106.86 Angstroms Squared	106.86 Angstroms Squared
Radius	5 Atom(s)	5 Atom(s)	5 Atom(s)
Shape Attribute	13.0666666666667	13.0666666666667	13.0666666666667
Shape Coefficient	0	0	0
Sum Of Degrees	28	28	28
Sum Of Valence Degrees	54	54	54
Topological Diameter	9 Bond(s)	9 Bond(s)	9 Bond(s)
Total Connectivity	0.0240562612162344	0.0240562612162344	0.0240562612162344
Total Valence Connectivity	0.000190181443578183	0.000190181443578183	0.000190181443578183
Wiener Index	414	414	414

Conclusion:

The present work reports conductivity data for pantothenic acid solutions in water, methanol at different temperatures, and mixtures of methanol & water, which were measured by using the lee-Wheaton equation at the best-fit values of standard deviation (σ Λ) for analyzing the data of symmetrical electrolytes . The values of conductivity parameters such as association constant Ka, Λo, and distance parameter R, differ from one solvent to another depending on the dielectric constant, viscosity, and interactions of the solution. These physical properties affected the Ka, Λo, values which reflect the thermodynamic parameters. the ΔH value of the compound in water is more than its value in methanol because the Ka value is more in water than in methanol (the Ka value in methanol is not systematically increasing or decreasing). when ΔH and ΔS are positive values it meant the process was endothermic and more random. ΔG was negative so spontaneous process.

Also, from theoretical results, the effect of the solvent property upon the Ka is in matching with the experimental results.

Acknowledgments:

The authors thank the University of Mosul, College of Science, Dept. of Chemistry, for give supporting this work.

References

[1] Scott, L. N., M. Fiume, et al. (2022). "Safety assessment of panthenol, pantothenic acid, and derivatives as used in cosmetics." International journal of toxicology 41(3_suppl): 77-128.

[2] Sanvictores, T. and S. Chauhan (2020). "Vitamin B5 (pantothenic acid)."

[3] Miller, J. W. and R. B. Rucker (2020). Pantothenic acid. Present knowledge in nutrition, Elsevier**:** 273-287.

[4] . Scholefield, M., S. J. Church, et al. (2021). "Substantively lowered levels of pantothenic acid (Vitamin B5) in several regions of the human brain in Parkinson's disease dementia." Metabolites 11(9): 569.

[5] Piquereau, J., E. Boitard, S., Ventura-Clapier, R., & Mericskay, M., 2021. Metabolic Therapy of Heart Failure: Is There a Future for B Vitamins?. ncbi.nlm.nih.gov (https://www.ncbi.nlm.nih.gov/pmc/articles/PMC8744601/)

[6] Bagotsky, V.S., *Fundamentals of electrochemistry*. 2005: John Wiley & Sons.

[7] Adekoya, O. C., G. J. Adekoya, et al. (2022). "Application of DFT calculations in designing polymer-based drug delivery systems: An overview." Pharmaceutics 14(9): 1972.

[8] Bursch, M., Mewes, J. M., Hansen, A., & Grimme, S. (2022). Best-practice DFT protocols for basic molecular computational chemistry. *Angewandte Chemie International Edition*, *61*(42), e202205735.

[9] F. M. Al-Healy and Y. Hameed, "Measurement of the Electrical Conductivity of Equivalent A number of Aspartic Acid Complexes in Different Percentages of Water Mixture with Methanol at 310 Absolute Temperature," Rafidain Journal of Science, vol. 29, no. 1, pp. 80–94, 2020, doi: 10.33899/rjs.2020.164483.

[10] Abdulrahmana Sh., Al-Healy F.,((2021) ,Electrical Conductance And Theoretical Study Of Glutamic Acid In Different Solvents at 310.16k, Egypt. J. Chem. Vol. 64, No. 8 pp. 4359 – 4367.

[11] Light T.S. ; (1984), Temperature dependence and measurement of resistivity of pure water, Analytical chemistry, 56,pp:1138

[12] PDe silva L.D., Freitas K.H.G and souse De F.F. ; (2017) , Electrical and dialectical properties of water, Scientiaplend, 13(1)

[13] Lee, W.H.; Wheaton, R.J.(1978) .Conductance of symmetrical, unsymmetrical and mixed electrolytes .J.C.S.Farady II,74,(pp.743-766).

[14] F. M. AL-HEALY,Y. O. HAMEED. Electrochemical and Thermodynamic Study of Tyrosine and its Complexes in Aqueous solution by conductivity measurement. (EPSTEM), 2019 Volume 7, Pages 48-57.

[15] Nancollas, G.H. (1966). "Interactions in Electrolyte Solutions". Elsevier, Amsterdam, Tables A-1 and A-5.

[16] Al-Healy,F., & Hameed, Y. (2020). Measurement of the Electrical Conductivity of Equivalent A number of Aspartic Acid Complexes in Different Percentages of Water Mixture with Methanol at 310 Absolute Temperature. Raf. J. Sci., 29(1), 80-94.

[17] Shahraki, M., Dehdab, M., & Elmi, S. (2016). Theoretical studies on the corrosion inhibition performance of three amine derivatives on carbon steel: Molecular dynamics simulation and density functional theory approaches. *Journal of the Taiwan Institute of Chemical Engineers*, *62*, 313-321.

[18] Singh, H., Singh, A., Banipal, T. S., Singh, P., & Bahadur, I. (2021). Temperature and concentration dependent physicochemical interactions of L-ascorbic acid in aqueous LiCl solution: Experimental and theoretical study. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, *623*, 126672.