



## Thermodynamic Study of the Solubility of Guanine and Uracil in Deferent Aqueous Sugar Solution

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### Abstract

We investigate the solubility of guanine and uracil, two nucleic acid bases xylose, glucose, and sucrose solutions in aqueous. It was discovered Guanine solubility rises in lockstep with glucose and sucrose concentrations. However, this is not the case for the other reagents. Guanine solubility increases below 1.5M reagent, and it follows this pattern: ribose(R) <xylose(X) <glucose (Glc) < sucrose(S). The ability to dissolve uracil in these solutions, and another hand, was dependent on the reagent, and it was observed that it decreased, increased, or remained unchanged. The temperature was found to play an important role in terms of the solubility of guanine and uracil in solutions containing sugar, and it was discovered that the transition of these molecules from the sugar solution to the water reaction was exothermic. We studied the solubility of the nucleic acid bases, Guanine and Uracil, in an aqueous sugar solution (glucose, xylose and sucrose) at three different temperatures (5, 25, and 45°C). The value of solubility  $S_v/S_o$  and equilibrium constant (K) were calculated and discussed. Thermodynamic parameters, i.e. change in standard free energy ( $\Delta G^0$ ), change in stander entropy ( $\Delta S^0$ ), energy transfer ( $\Delta G_{tr}$ ), and change in standard enthalpy ( $\Delta H^0$ ) for all these compounds were also calculated and discussed.

*Keyword:* solubility; guanine; uracil, xylose; glucose, sucrose

### 1. Introduction

Purines and pyrimidine's are two types of purines that are important in terrestrial biology. Adenine, guanine, cytosine, thymine, and uracil aromatic ring structures that contain nitrogen (N-heterocyclic) are examples of purines. Nucleus bases are ubiquitous and ancient in biochemistry, as evidenced by their importance in coenzymes and biochemical pathways. They are used to provide information. Ribonucleic acid (RNA) and deoxyribonucleic acid (DNA) monomers (DNA) that lack Groups of sugar and phosphate (DNA) (Bloch,1996 ) In terrestrial life, guanine and adenine are found in both RNA and DNA, uracil is only found in RNA, and thymine is only found in DNA. Both endogenous and exogenous sources affect the use of nucleus bases as a feedstock for prebiotic chemistry, which results in the early the first self-replicating structures on Earth to see whether exogenous purines and pyrimidine's are abundant on prebiotic Earth.[1] Guanine's peculiar behavior obscured its dissolution in neutral solutions,

implying that solubility is clearly dependent on the amount of solid guanine used The problem is caused by the formation of nanoparticles of guanine., which eventually transform into stable calcium particles., as seen here. Dimensions: 800 nanometers. This impact has the potential to be minimized. Tiny amounts of guanine powder were used for dissolution. Furthermore, it is shown that assuming a fixed value, pH-independent guanine nucleotide concentration of 25.4 M at 25°C For dissociation or protonation, established pKa values are used. It is possible to measure guanine's solubility by measuring the levels of concentrations of both acids that are conjugated and bases of guanine at the specified pH level.[2] In RNA, the 2'-OH sugar and the methyl group in dT (for example, 5-methyl-dU). are the major chemical distinctions between DNA and RNA The sugar discrepancy chemistry is primarily responsible for DNA and RNA's very different solution aqueous conformations; the conformation of C3'-endo sugar is stabilized by C2'-OH is present in RNA. While the 2'-deoxy sugar DNA conformation The C2'-endo

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conformation is the most common. s. The methyl group of dT, on the other hand, tends to have the greatest impact on DNA's thermodynamic stability[3, 4]. At 298, 308, and 318 K, Uracil in urea aqueous solution 1: volumetric, viscometric, and ultrasonic measurements were performed at concentrations of 2, 3, and 5 M. In an aqueous urea solution, the uracil concentration varies from 0.05 to 0.4 percent. Measurements were made for density ( $\rho$ ), viscosity and sound speed ( $u$ ). Various thermodynamic and acoustic parameters are computed using the experimental data. The results were explored in terms of solute-solute and solvent-solvent interactions, as well as structural differences in solutes in solutions. Temperature variation's effect on these interactions has also been investigated[5].

## 2. Experimental

### 2.1. Materials

We used BDH, Pool, U.K.'s chromatographic grade guanine (G) and uracil (U). For these compounds, the solubility step curves revealed impurities are not present in large quantities; after distillation from all glass cells, Merck's PH of xylose and ribose The PH of the glucose and sucrose water used was 6.

### 2.2. Measurements of Solubility:

In an incubator, a shaker (New Brunswick Scientific Co. is a company based in New Jersey.), the solutions were equilibrated at 25 percent, 45 percent, and 47 percent in 10ml screw-capped tubes. The 5Co equilibration was done in tubes with screw caps lined with Teflon that were immersed in a bath of water in a cold setting on a rotating rack. End over end rotation of the tubes was used to blend the contents. At higher temperatures, the equilibration time was 48 hours, and at 5 degrees Celsius, it was 72 hours. Calculating the concentration of solutes in solutions at various equilibration points, the achievement of equilibrium was confirmed.[6]. at or above the equilibration temperature, the equilibrated solution is filtered, and the liquids are sampled after proper solution, the Solute concentrations. was measured by calculating the absorbance of the solution, at 240 and 251nm for (G) and (U) The extinction values of mar, on the other hand, were  $13.1 \times 10^{-3}$  at 240 nm for (G) and  $7.6 \times 10^{-3}$  at 251 nm for (U) According to the literature, the values are  $13.3 \times 10^{-3}$  and  $7.8 \times 10^{-3}$ , respectively[7] We believed that since water solubility values is repeatable to a

precision of 5 %, the same range of experimented error extended to determination in other solvents.

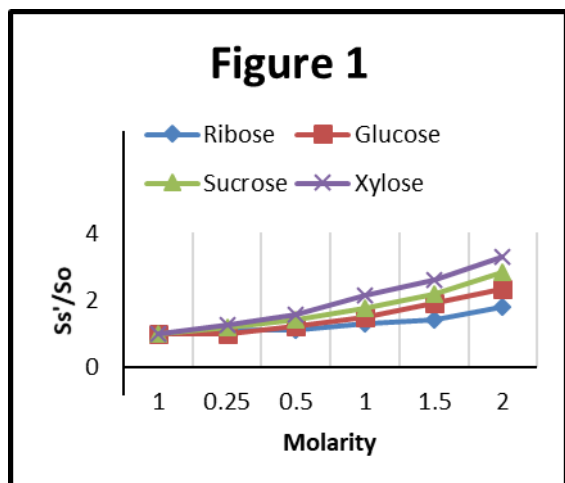
## 3. Results.

Table 1 shows the solubility of G and U in various solutions. Below 1.5M reagent concentration, in glucose and sucrose (Figure 1, Ss and So are the qualities of solubility in sugar solution and water, respectively), a linear increase in G solubility is observed, as well as a nonlinear rise in xylose (the results for ribose and xylose are identical, see Table 1) and solution. The solubility of G increases as the sequence progresses, while xylose (ribose) and glucose solubility remain unchanged. In the presence of sugar. However, the solubility of U is virtually unchanged. The effect of bases' self-association their soluble nature was not established. However, it was supposed to be minor ranges of concentrations of the bases studied. This means the interaction between oneself and another will have no effect on the solubility value mentioned here[7]. Without it, dynamic precipitation of a complex during solid solution formation, thorough microscopic examination of the solid phases G and U reveals no changes in the structure of the solid phase[8, 9] which may have influenced the outcomes mentioned here. From  $\Delta G_{tr} = -RT \ln Ss'/So$  (C. Nick Pace & Saul Trevin2004), the amount of transferring free energy  $\Delta G_{tr}$  = from water to different reagent solutions, have been determined and are reported in Table 2 for two different sugar concentrations and temperatures. Figure 2 depicts the influence of temperature on the  $\Delta G_{tr}$  value of G in a solution of glucose. Sugar solutions communicate with each other more effectively than water, and the reaction is exothermic.

**Table 1.** Solubility of guanine and uracil in various solvents (M  $10^3$ )

solvents	Guanine					Uracil				
	0.25 M	0.5 M	1 M	1.5 M	2 M	0.25 M	0.5 M	1 M	1.5 M	2 M
Ribose	0.92	1.1	1.2	1.5						
Xylose	1.05	1.8	2.2	2.84	3.66	4.11	5.14	3.01	3.64	
Glucose	0.88	1.26	1.49	1.59	4.31	4.25	4.14	4.10	3.90	
Sucrose	1.0	1.5	1.84	2.4	4.12	4.45	4.34	4.09	3.93	
Water						3.76 $\pm$ 0.02b (25 °C)				
	0,84 $\pm$ 0.02 b					4.20 $\pm$ 0.02b (30 °C)				

A) At 25°C, with the exception of guanine in ribose, which is at 24°C, and uracil in glucose and sucrose at 30°C. ? So, at 24°C, 0.84 $\pm$  0.02 for guanine  
B) The standard deviation of the mean

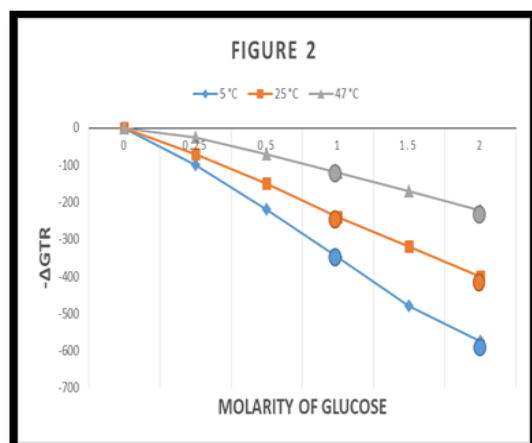


**Figure 1.** shows the rise in guanine solubility as the reagent concentration is increased at 25°C. The solubility's in sugar solution and water are described by the quantities  $Ss'$  and  $So$  respectively.

**Table 2.** The free energy of transition,  $\Delta G_{tr}$  of guanine and uracil from various solvents at different temperatures

Comp.	Temp.	Glucose		Xylose		Sucrose	
		1M	2M	1M	2M	1M	2M
Guanine	5°C	-350	-575	-287	-665	-492	-745
	25°C	-240	-400	-189	-432	-397	-729
	45°C	-120 b	-222 b	-146 b	-298 b	-368	-584
Uracil	5°C	10	-21			0	-45
	25°C	26	64	-174	-12	0	57
	45°C	66	123			93	185

A) The free energy of transfer values for Guanine is measured using the determined solvent values of  $1.41 \cdot 10^{-2}$  and  $0.37 \cdot 10^{-2}$  M at 47 and 5 degrees Celsius, respectively. At 45°C and 5°C, the values for uracil are  $5.13 \cdot 10^{-2}$  and  $1.22 \cdot 10^{-2}$  M, respectively. The values are in call  $\text{mol}^{-1}$  measured as defined in the text.



**Figure 2.** Guanine transfer's free energy,  $\Delta G_{tr}$ , from water to various glucose concentrations at three different temperatures.

Increased  $\Delta G_{tr}$  with increased temperature also reveals the exothermic presence of Uracil in sucrose

and glucose solution. Dissolving G in glucose solution clearly in valves some kind of energy release (if the temperature increases, the negative kinetic energy of the molecules in the solution also increases). In fact, all of these compounds are highly soluble in water, the  $\Delta G$  for the formation at all solution is negative, but the process results in different temperature changes. In different concentration the interactions after the solution are formed are strong and more stable.

The enthalpy is the amount of internal energy contained (in a compound whereas. and the entropy measures the amount of heat dispersed or transferred during the chemical process (measure degree of randomness). The process of dissolving increases the entropy because the solute partial become separated from the phase. Entropy increases as temperature increases because particles of the substance have greater kinetic energy. In Table 3 and 4, vales were calculated and discased.

The enthalpy  $\Delta g$ , and entropy  $\Delta S$  is endothermic because energy must be supplied against the cohesive force of the solvent. This process decrease solubility. On the other hand, the enthalpy of solute- solvent interaction is exothermic and results mainly from Vander Waals and Lewis acid- bases interaction. Thus, the negative values obtained for enthalpy and entropy of mixing Guanine and uracil in solvents solute molecules have migrated from the dipolar organic phase in the sugar solution become occupied by sugar molecules. This event produces an energy release due sugar- sugar interaction. Thus the negative enthalpy values of transfer obtained could be explained by strong interaction due to hydrogen-bonding.

**Table 3.** Thermodynamic Parameters of Guanine in different solvents at 25°C

Solvent	M	$\Delta G^\circ$ Kcal. mol <sup>-1</sup>	$\Delta H^\circ$ Kcal mol <sup>-1</sup>	$\Delta S^\circ$ cal.mol <sup>-1</sup> K <sup>-1</sup>	T $\Delta S$ Kcal. mol <sup>-1</sup>
Glucose	M1	+0.076a	-12.477	-41.264	12.477
	M2	+0.064a	+2.374	+7.623	2.31
Xylose	M1	0.174	----	-----	-----
	M2	0.012	----	-----	-----
Sucrose	M1	0	0	0	
	M2	+0.057	+1.676	+5.432	1.619

A)  $\Delta G^\circ$  calculates by the equation as follows:

$$\Delta G^\circ = -R T \ln k$$

B)  $\Delta H^\circ$  and  $\Delta S^\circ$  calculates by Vont Half equation as follows:  $\frac{\ln k_1}{T_1} = \frac{-\Delta H^\circ}{R} + \frac{\Delta S^\circ}{R T_1}$

$$\left( \frac{1}{T_1} - \frac{1}{T_2} \right)$$

C)  $\Delta G^\circ = \Delta H^\circ - T \Delta S^\circ$

D) Reference for equations (Perrot, Pierre (1998) .Atos Thermodynamic oxford University)

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**Table 4.**  
Thermodynamic Parameters of Uracil in different solvents at 25°C

Solvent	M	$\Delta G^\circ$	$\Delta H^\circ$	$\Delta S^\circ$	T $\Delta S$
		Kcal. mol <sup>-1</sup>	Kcal mol <sup>-1</sup>	cal.mol <sup>-1</sup> K <sup>-1</sup>	Kcal. mol <sup>-1</sup>
Glucose	M1	-0.24	-3.110	-9.630	2.87
	M2	-0.4	-3.051	-8.775	2.615
Xylose	M1	-0.189	-3.233	-10.244	3.053
	M2	-0.146	-4.668	-15.080	4.494
Sucrose	M1	-0.492	-2.639	-8.211	2.447
	M2	-0.748	-2.707	-6.573	1.959

A) values are at 25°C

#### 4. Discussion

We have noticed that  $-\Delta G_{tr}$  (transfer's free energy) values for G from water to sugar solutions could indicate a reduction in G's between the reagents forming a stoichiometric complex, or both[10]. Never the less, the debate that follows will be focused solely on the free energy of transition. We can characterize nucleic acid bases as cyclic amides. Isopeistic vapor pressure measurements indicate that their favorable interaction of sucrose with G is close to another favorable interaction between sucrose and amides[11]. Features of the interaction found here are similar to those observed in interactions between those bases and steroids[12], as well as the nucleic acid bases. Additionally we observed that the relationship between purine and sugar is greater than which appears to be similar to purine-purine metrication > interaction between pyrimidine and pyrimidine[13].

G considerate amount of studies was based on the Physic-chemical Aspects of Sugar Aqueous Solutions focusing mainly on the basis of their apparent molar volume Sugar molecule compressibility and hydration[14, 15].

As we found out in previous studies, a reduction in water activity or a reduction in the study's sugar solubility cannot be clarified.

We discovered that the differential nature of G and U solubility in sugar solutions cannot be explained because it is caused by the above effects: decreased dipole-dipole interaction of the bases with sugar molecules in solution and their increased solubility[16]. the disparity in solubility activity of G and U in these solutions cannot be explained by dipole-dipole interactions.

In the presence of other co-solvents, the H-bond density in water decreases, making it easier to position any molecule in the aqueous solutions of the co-solvent.[9] Since Taylor and Rawlinson's calorimetric proof, is not to blame for G's increased

solubility[17] and showed that in aqueous sugar solutions, the density and strength of the H-bond increases. Moreover, compared to water–water, there was a decrease in the density of H-bonding and a rise in H-bonds between sugar and water. H-bonds were thought to be the cause of model peptides' decreased solubility in sugar solutions, observe the outcomes of the sugar solutions in these studies are related to Increase the intensity of its limits or the number of them, as it would be more energetically difficult to position any molecules., compared to water in sugar solutions. This unfavorable energetic of interaction is properly regulated in the case of G by G's favorable interaction (polar) with a solvent, while this is not possible in the case of U The exothermic nature of both bases' interactions with sugar in sugar solutions most likely means that the water base H-bond has been replaced by the sugar base H-bond.

The unfavorable effect is influenced by the solvent's polar interaction with G, which is likely attributable to G has more H–bonding sites than U, which influences the polar interaction due to the unfavorable interaction.

Furthermore, Stereo chemical res eviction interaction of H-bonds in U may be to blame for too much interaction that is beneficial forming. It's likely that interaction polar occurs at the molecules' periphery, while interaction that is unfavorable occurs at the planar surface molecules', With G and temperature. In sugar solution, the unfavorable positive free energy of transfer of N-acetyl L-phenylalanine ethyl ester increases.as previously demonstrated. The decreased  $\Delta G$  with G and increased positive  $\Delta G_{tr}$  with U- $\Delta G$  TV sugar solution is most likely because of polar interaction's exothermic existence as well as the increased interaction between the sugar molecules in solution and the base relative to water. We will illustrate these findings using glucose and sucrose because we believe they would apply to other systems studied here[18].

We already discussed that the overall existence of the sugar–guanine and sugar–uracil interactions, in terms of free energy, is identical Purine–purine and pyrimidine–pyrimidine also the purines and pyrimidine's, interactions, respectively.

It's likely that the relationship between sugar and base will conflict using a vertical stack in nucleic acid base interactions. As proof needed by calorimetric measurements, Will et al[19] indicated

that adding the stacking conformation is influenced by the nucleic acid base's sugar moiety. Sugar-guanine and sugar-uracil interactions are also strikingly similar to purine nucleotide and pyrimidine nucleoside self-association[19, 20].

The possibility of striking a compromise between sugar-pyrimidine (unfavorable) inspiration in eviction, Self-association of pyrimidine nucleosides and beneficial sugar-purine interactions are essential. Self-association of purine nucleosides has been suggested as a factor influencing nucleic acid helix stability under various conditions of the solution.

## 5. Conclusions

The solubility of guanine and uracil in aqueous solutions on different sugars was studied, in order to comprehend the mechanism by which these bases and sugar molecules interact. Future research will benefit greatly from the solubility of nucleic acid bases in sucrose solution-base studies in this study. where it was observed that the solubility guanine of increased linearly in aqueous solutions of glucose and sucrose, and a non-linear increase with the aqueous solution of xylose sugar, while the solubility of uracil remained practically unaffected by the presence of sugar. The effect of self-association of bases and their solubility was not determined, but it was expected to be small in the range of concentrations of the studied bases and this indicates that the self-reaction will not affect the solubility value. We have observed that the differential nature of G and U solubility in sugar solutions cannot be explained as it's resulting from a decrease in water activity effects the decreased dipole- dipole interaction of the bases with sugar molecules in solution and their increased dipole-dipole interaction with each other cannot explain the difference in the solubility behavior of G and U in these solutions. The decreased  $\Delta G$  with G and increased positive  $\Delta G_{tr}$  with U- $\Delta G$  TV sugar solution is most likely due to the exothermic nature of polar interaction as well as the increased interaction between the base and sugar molecules in solution relative to water. The transfer process between G and U and sugar solution with hydrogen-bonding capability as dipole-dipole or acceptor or donors interaction ,the entropic and enthalpy changes imply energetic requirements and the molecular random (decrease or increase in the molecular), respectively. The thermodynamic parameters  $\Delta G$ ,  $\Delta S$ ,  $\Delta H$  calculated and diseased.

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