https://dx.doi.org/10.22161/ijaems.4.11.7 ISSN: 2454-1311

Demonstration of the Formation of the Caffeine-Dichloromethane-water Emulsion using Quantum Chemistry

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***Abstract*— *Researchers have been concerned with the subsequent study of caffeine extraction. The objective of this article was to demonstrate how the caffeine-dichloromethane-water emulsion is formed. We use the theory of the electron transfer coefficient (ETC) as the cornerstone of our research. All the simulations of the interactions of the substances involved were calculated with the hyperchem simulator. The emulsion is formed because the ETC = 36,196 of the caffeine-CH_2Cl_2 interaction is the lowest of the cross-band interactions of the mixture. It will expect massive amounts of caffeine emulsified with CH_2Cl_2 and water. In conclusion, the gravitational well and the quantum well of caffeine coincide in being the lowest of all the wells calculated. It means that both CH_2Cl_2 and H_2O will not destroy caffeine. That is, caffeine will be kept as a pure substance even after extraction with these two solvents. Although CH_2Cl_2 extracts more caffeine, due to its low ETC, the product for human consumption can be contaminated.*

Keywords*— *Caffeine, Dichloromethane, Water, Emulsion, Quantum Chemistry

I. INTRODUCTION

Researchers have been concerned with the subsequent study of caffeine and catechins in the biomass of green tea using an optimized SFE (supercritical fluid extraction) method. The SFE of caffeine was carried out at different pressures (10, 20, 25, 30 MPa), temperature (30, 40, 50, 60 ° C) and extraction periods (1, 2, 3, and five h) for 10 g of sample. Caffeine extract yields and purity were optimized for successful separation. Optimal conditions for the extraction of caffeine were 25 MPa of pressure at 60 ° C for three h of extraction period. [1-3]

In other experiment investigators extracted caffeine with CHCl3 from the aqueous solution obtained by treating guarana powder with HCl, followed by filtration and alkalization. Using the melting point and thin layer chromatography, they verified the purity of the isolated caffeine. [4]

A sequential statistical mixture allowed the optimization of extraction systems and mobile phase solvents to increase the differences detected in the metabolites of plants. [5-9]

The objective of this article was to demonstrate how the caffeine-dichloromethane-water emulsion is formed using calculations made with the hyperchem simulator.

II. MATERAILS Y METHODS

We use the theory of the electron transfer coefficient as the cornerstone of our research. All the simulations of the interactions of the substances involved were calculated with the hyperchem simulator. We use the semi-empirical method PM3 specifically.

It has used this methodology in many projects carried out and published. [10-16]

III. RESULTS AND DISCUSSIONS

Table 1 shows an extract from table 2. It shows the ETCs of pure substances in descending form according to the depth of the quantum wells. It can be noted that caffeine is the most stable substance of all because it is in the deepest well.

Table 1. ETCs of pure substances

Number	Reducing agent	Oxidizing agent	ETC
1	CH_2Cl_2	CH_2Cl_2	76.048
2	H_2O	H_2O	54.950
3	Caffeine	Caffeine	31.933

These ETCs were extracted from table 2 (below)

Table 2 shows all the possible interactions taken from two in two of these three pure substances. Interaction 9 has an ETC = 31.933. This value is the lowest of the nine

https://dx.doi.org/10.22161/ijaems.4.11.7 ISSN: 2454-1311

calculated interactions and tells us that caffeine is the most stable substance.

The other interactions are given according to their depth in the quantum well; they increase their instability until they reach the number CH_2Cl_2-H_2O. The most unstable substance is the substance with the highest energy.

Figure 1, shows us the difference between the ETC of CH_2Cl_2 and caffeine is 44.115 units of ETC. The CH_2Cl_2 is unstable; moreover, it falls to the bottom of the caffeine well and rises to it forming a new interaction of 4.263 units above. This new Caffeine-CH_2Cl_2 interaction has an ETC of 36.196. In this new interaction, CH_2Cl_2 remains as an oxidizing agent of caffeine.

The different interaction was calculated, where caffeine is an oxidizing agent; ETC = 67.721. Because nature always seeks the least energy, CH_2Cl_2 is more likely to be the oxidizing agent. The zone in which the two interactions of CH_2Cl_2-Caffeine, Caffeine-CH_2Cl_2, are located is of average probability. That is, they do not go beyond the limits of their pure substances

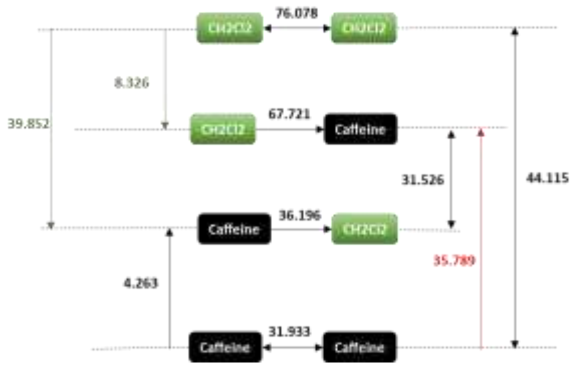

Fig. 1 Measures of the ETCs of the quantum well of the interaction caffeine and CH_2Cl_2.

Figure 2, show us the difference between the ETC of H_2O and caffeine is 23.017 units of ETC. As H_2O is unstable, it drops to the bottom of the caffeine well and rises it forming a new interaction of 11.087 units above. This new Caffeine-H_2O interaction has an ETC of 43.019. In this new interaction, H_2O remains as an oxidizing agent of caffeine.

The different interaction was calculated, where caffeine is an oxidizing agent; ETC = 45.479. Because nature always seeks the lowest energy, that is, the deepest well, H_2O is more likely to be the oxidizing agent. The zone in which the two H_2O interactions-Caffeine, Caffeine-H_2O are located is of medium probability. That is, they do not go beyond the limits of their pure substances.

By the way, we describe the two solvents and their interactions with caffeine; because the interaction pattern is identical, only the ETC values change.

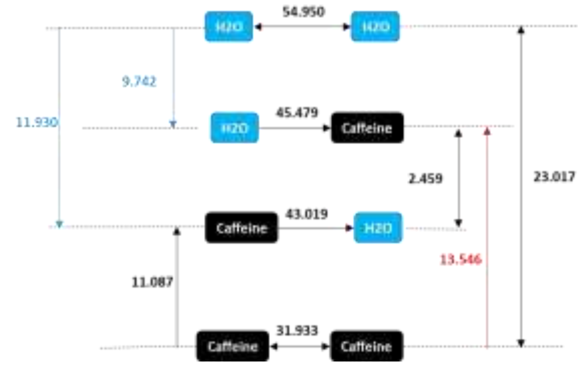

Fig. 2 Measures of the ETCs of the quantum well of the interaction caffeine and water.

In Figure 3, a different pattern of the H_2O-CH_2Cl_2 mixture can be observed. In this case, the H_2O-CH_2Cl_2 interaction has the lowest ETC. In contrast, the inverse interaction goes out of the upper limit. Therefore, the CH_2Cl_2-H_2O interaction falls in the area of least or nil probability. With these observations we can launch two hypotheses.

H1 "CH_2Cl_2 is an oxidizing agent of H_2O. H_2O cannot be an oxidizing agent of CH_2Cl_2."

H2 "CH_2Cl_2 highly soluble in water"

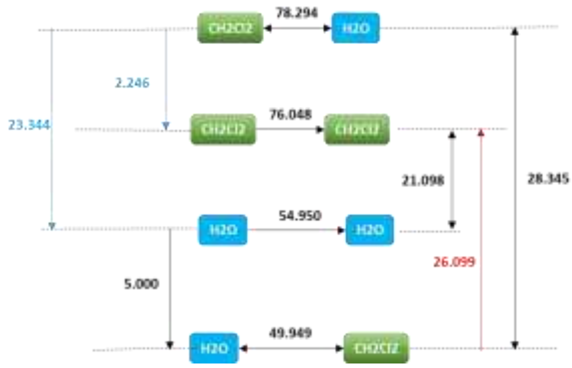

Fig. 3 Measures of the ETCs of the quantum well of the interaction dichloromethane and water.

We went to the laboratory to check our hypothesis. We find some controversies.

In Figure 4, a mixture of caffeine + CH_2Cl_2 + H_2O is shown. In it, an unexpected emulsion is observed. The first time the emulsion is very homogeneous. In the second moment, it was left to rest, and two distinct phases were observed.

The bottom phase has an emulsion, and in the upper part, only a caffeine solution with water is shown.

We made a mixture of H_2O-CH_2Cl_2 shown in figure 5. In this figure, it can be seen that the CH_2Cl_2 was located at the bottom of the flask and the H_2O above. This phenomenon occurs due to the gravitational field since CH_2Cl_2 is heavier than H_2O.

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Fig. 4 CH2Cl2+H2O+Caffeine. A) Freshly stirred mixture. B) Relaxed mix

Hypothesis 2 is not fulfilled. There is no solution; there are two phases in the flask. With this observation, it can be said that the gravitational well predominated over a quantum well. However, due to the lower ETC of the H_2O-CH_2Cl_2 interaction, the interface of this mixture is powerful.

Fig. 5 Mixture of H_2O + CH_2Cl_2

Why an emulsion?

The emulsion is formed because the ETC = 36,196 of the caffeine-CH_2Cl_2 interaction is the lowest of the cross-band interactions of the mixture. Expect copious amounts of caffeine emulsified with CH_2Cl_2 and water. In other words, caffeine is entrained by the CH_2Cl_2 at the bottom of the flask due to the molecular weight of both. They do not separate due to their lower ETC of the crossed bands (Table 3).

In contrast, the CH_2Cl_2-H_2O interaction has a lower ETC of its binary mixture. Therefore, it also sticks to caffeine forming a trio. It can be said that the caffeine molecule acts as an emulsifying agent (or coupling agent) of CH_2Cl_2 and H_2O.

Why Caffeine-H_2O solution?

The ETC = 43.019 is the lowest of the caffeine mix with H_2O traps caffeine in the water. They are located above the emulsion due to the molecular mass of the interaction.

Table 3. Quantum well (ETC) and gravitational well (Total mass)

Number	Reducing agent	Oxidizing agent	ETC	Total mass
1	CH_2Cl_2	H_2O	78.294	102.933
2	CH_2Cl_2	CH_2Cl_2	76.048	169.866
3	CH_2Cl_2	Caffeine	67.721	279.123
4	H_2O	H_2O	54.950	36
5	H_2O	CH_2Cl_2	49.949	102.933
6	H_2O	Caffeine	45.479	212.19
7	Caffeine	H_2O	43.019	212.19
8	Caffeine	CH_2Cl_2	36.196	279.123
9	Caffeine	Caffeine	31.933	388.38

IV. CONCLUSION

The gravitational well and the quantum well of caffeine coincide in being the lowest of all the wells calculated. It means that both CH_2Cl_2 and H_2O will not destroy caffeine. That is, caffeine will be kept as a pure substance even after extraction with these two solvents (ETC = 33,933). On the other hand, due to its mass and the gravitational well, the caffeine will precipitate in any of the solvents.

Although CH_2Cl_2 extracts more caffeine, due to its low ETC = 36.196, the product for human consumption can be contaminated.

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Table 2. Cross-band ETCs of the 3 compounds involved in this investigation. These ETCs are ordered from highest to lowest according to the depth of your quantum well.

Number	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	E-	E+	EP	ETC
1	CH_2Cl_2	H_2O	-10.582	4.059	14.641	-0.016	0.171	0.187	78.294
2	CH_2Cl_2	$CH2Cl_2$	-10.582	0.521	11.103	-0.016	0.130	0.146	76.048
3	CH_2Cl_2	Caffeine	-10.582	-0.491	10.091	-0.016	0.133	0.149	67.721
4	H_2O	H_2O	-12.316	4.059	16.375	-0.127	0.171	0.298	54.950
5	H_2O	CH_2Cl_2	-12.316	0.521	12.837	-0.127	0.130	0.257	49.949
6	H_2O	Caffeine	-12.316	-0.491	11.825	-0.127	0.133	0.260	45.479
7	Caffeine	H_2O	-8.890	4.059	12.949	-0.130	0.171	0.301	43.019
8	Caffeine	$CH2Cl_2$	-8.890	0.521	9.411	-0.130	0.130	0.260	36.196
9	Caffeine	Caffeine	-8.890	-0.491	8.398	-0.130	0.133	0.263	31.933