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-CH₂Cl₂ interaction is the lowest of the cross-band interactions of the mixture. It will expect massive amounts of caffeine emulsified with CH₂Cl₂ 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 CH₂Cl₂ and H₂O will not destroy caffeine. That is, caffeine will be kept as a pure substance even after extraction with these two solvents. Although CH₂Cl₂ 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. MATERIALS 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.

| Number | Reducing agent | Oxidizing agent | ETC  |
|--------|----------------|----------------|------|
| 1      | CH₂Cl₂         | CH₂Cl₂         | 76.048|
| 2      | H₂O            | H₂O            | 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
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 \( \text{CH}_2\text{Cl}_2 - \text{H}_2\text{O} \). The most unstable substance is the substance with the highest energy.

Figure 1, shows us the difference between the ETC of \( \text{CH}_2\text{Cl}_2 \) and caffeine is 44.115 units of ETC. The \( \text{CH}_2\text{Cl}_2 \) 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-\( \text{CH}_2\text{Cl}_2 \) interaction has an ETC of 36.196. In this new interaction, \( \text{CH}_2\text{Cl}_2 \) 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 lowest energy, that is, the deepest well, \( \text{H}_2\text{O} \) is more likely to be the oxidizing agent. The zone in which the two interactions of \( \text{CH}_2\text{Cl}_2 \)-Caffeine, Caffeine-\( \text{CH}_2\text{Cl}_2 \), are located is of average probability. That is, they do not go beyond the limits of their pure substances.

In Figure 3, a different pattern of the \( \text{H}_2\text{O}-\text{CH}_2\text{Cl}_2 \) mixture can be observed. In this case, the \( \text{H}_2\text{O}-\text{CH}_2\text{Cl}_2 \) interaction has the lowest ETC. In contrast, the inverse interaction goes out of the upper limit. Therefore, the \( \text{CH}_2\text{Cl}_2 - \text{H}_2\text{O} \) interaction falls in the area of least or nil probability. With these observations we can launch two hypotheses.

H1 “\( \text{CH}_2\text{Cl}_2 \) is an oxidizing agent of \( \text{H}_2\text{O} \). \( \text{H}_2\text{O} \) cannot be an oxidizing agent of \( \text{CH}_2\text{Cl}_2 \).”

H2 “\( \text{CH}_2\text{Cl}_2 \) highly soluble in water”

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

In Figure 4, a mixture of caffeine + \( \text{CH}_2\text{Cl}_2 \) + \( \text{H}_2\text{O} \) 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.

We made a mixture of \( \text{H}_2\text{O}-\text{CH}_2\text{Cl}_2 \) shown in figure 5. In this figure, it can be seen that the \( \text{CH}_2\text{Cl}_2 \) was located at the bottom of the flask and the \( \text{H}_2\text{O} \) above. This phenomenon occurs due to the gravitational field since \( \text{CH}_2\text{Cl}_2 \) is heavier than \( \text{H}_2\text{O} \).
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 H₂O-CH₂Cl₂ interaction, the interface of this mixture is powerful.

Why an emulsion?
The emulsion is formed because the ETC = 36,196 of the caffeine-CH₂Cl₂ interaction is the lowest of the cross-band interactions of the mixture. Expect copious amounts of caffeine emulsified with CH₂Cl₂ and water. In other words, caffeine is entrained by the CH₂Cl₂ 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 CH₂Cl₂-H₂O 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 CH₂Cl₂ and H₂O.

Why Caffeine-H₂O solution?
The ETC = 43.019 is the lowest of the caffeine mix with H₂O 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      | CH₂Cl₂         | H₂O             | 78.294| 102.933    |
| 2      | CH₂Cl₂         | CH₂Cl₂          | 76.048| 169.866    |
| 3      | CH₂Cl₂         | Caffeine        | 67.721| 279.123    |
| 4      | H₂O            | H₂O             | 54.950| 36         |
| 5      | H₂O            | CH₂Cl₂          | 49.949| 102.933    |
| 6      | H₂O            | Caffeine        | 45.479| 212.19     |
| 7      | Caffeine       | H₂O             | 43.019| 212.19     |
| 8      | Caffeine       | CH₂Cl₂          | 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 CH₂Cl₂ and H₂O 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 CH₂Cl₂ 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      | CH2Cl2         | H2O             | -10.582 | 4.059 | 14.641 | -0.016 | 0.171 | 0.187 | 78.294 |
| 2      | CH2Cl2         | CH2Cl2          | -10.582 | 0.521 | 11.103 | -0.016 | 0.130 | 0.146 | 76.048 |
| 3      | CH2Cl2         | Caffeine        | -10.582 | -0.491 | 10.091 | -0.016 | 0.133 | 0.149 | 67.721 |
| 4      | H2O            | H2O             | -12.316 | 4.059 | 16.375 | -0.127 | 0.171 | 0.298 | 54.950 |
| 5      | H2O            | CH2Cl2          | -12.316 | 0.521 | 12.837 | -0.127 | 0.130 | 0.257 | 49.949 |
| 6      | H2O            | Caffeine        | -12.316 | -0.491 | 11.825 | -0.127 | 0.133 | 0.260 | 45.479 |
| 7      | Caffeine       | H2O             | -8.890 | 4.059 | 12.949 | -0.130 | 0.171 | 0.301 | 43.019 |
| 8      | Caffeine       | CH2Cl2          | -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 |