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ANALYSIS OF THE CHEMICAL-QUANTUM INTERACTIONS OF FIVE ORGANIC SOLVENTS AND THEIR RELATIONSHIP WITH THEIR QUANTUM MOLECULAR IMPEDANCES RELATIVE TO WATER

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ABSTRACT

The use of polar protic, aprotic solvents and apolar solvents are essential for the study of the extraction and reaction of substances with biological activity. The objective of this study was to analyze the chemical-quantum interactions of five solvents. From this analysis, it was determined if the phases are miscible or immiscible. We use hyperchem simulator to perform the quantum calculations of the related variables in question. Of the results obtained, only the gravitational wells are predominant to the quantum well, as long as the mass difference is enormous.

INTRODUCTION

The use of polar protic, aprotic solvents and apolar solvents are essential for the study of the extraction and reaction of substances with biological activity. [1-3] Dichloromethane, ethyl acetate and methanol are frequently used solvents due to their chemical characteristics. [4-11] These solvents are very important for the medicine and treatment of diseases, for example, Castro (1999) evaluated the organic extracts in tropical plants with the ability to neutralize the hemorrhagic activities induced by the venom of the snake Bothrops asper. This researcher concluded that the total inhibition of hemorrhage occurs with ethanolic, ethyl acetate and aqueous extracts. [12, 13] On the other hand, Martinez (2003) evaluated the efficiency of the extract of the Cactus lefaria as a coagulating agent in the clarification process and used methanol, ethyl acetate and petroleum ether for the extraction of cactus lefaria. He obtained the best values of turbidity when treating the Cactus lefaria with methanol and ethyl acetate for initial turbidity of turbid water of 20 and 30 NTU. [14]

MATERIALS AND METHODS

General equations [15]:

We did the bandgap calculations first:

$$BG = |HOMO - LUMO| \quad (1)$$

Where: HOMO is Highest Occupied Molecular Orbital. LUMO is Lowest Unoccupied Molecular Orbital. BG is BandGap.

In the second place we made the calculations of the electrostatic potential:

$$EP = |E_- + E_+| \quad (2)$$

Where: E- is the negative electrostatic potential of the molecule. E+ is positive; and, EP is the absolute value of the difference of both potential.

In third place we did the ETC calculations:

$$ETC = \frac{BG}{EP} \quad (3)$$

In four place we did the GW:

$$GW = m_1 + m_2 \quad (4)$$

Where: m1 is the molecular mass of molecule 1; m2 is the molecular mass of molecule 2; and, GW is the Gravitational Well.

Parametrization of the hyperchem software [16-21]:

Table 1. Parameters used for quantum computing molecular orbitals: HUMO and LUMO

Parameter	Value	Parameter	Value
Total charge	0	Polarizability	Not
Spin Multiplicity	1	Geometry Optimization algorithm	Polak-Ribiere (Conjugate Gradient)
Spin Pairing	RHF	Termination condition RMS gradient of	0.1 Kcal/Amol
State Lowest Convergent Limit	0.01	Termination condition or	1000 maximum cycles
Interaction Limit	50	Termination condition or	In vacuo
Accelerate Convergence	Yes	Screen refresh period	1 cycle

Table 2. Parameters used for visualize the map of the electrostatic potential of the molecules

Parameter	Value	Parameter	Value
Molecular Property	Property Electrostatic Potential	Contour Grid increment	0.05
Representation	3D Mapped Isosurface	Mapped Function Options	Default
Isosurface Grid: Grid Mesh Size	Coarse	Transparency level	A criteria
Isosurface Grid: Grid Layout	Default	Isosurface Rendering: Total charge density contour value	0.015
Contour Grid: Starting Value	Default	Rendering Wire Mesh	

RESULTS AND DISCUSSION

It is observed in table 3 that hexane has the highest value of ETCs of all the pure substances in question. Also, ethanol-dichloromethane interaction has a lower ETC value than the entire calculated table; therefore, this interaction is the one that has a lower impedance or greater conductance and is the most probable or stable.

Quantum molecular impedance relative to water (QMIRW) and Quantum molecular conductance relative to water (QMCRW) is two new concepts. These concepts are similar to impedance and conductance in electronic science. We can observe, hexane has the highest QMIRW; while interaction ethanol-dichloromethane as the lowest.

The last three interactions 23, 24, and 25; show as that these three substances have a high probability of being soluble in dichloromethane table 4.

In table 4, we can see four sub-tables of the combinations of dichloromethane mixed with other solvents. The four sub-tables have a similar pattern. The deepest quantum wells are placed at the gravitational well interface (columns 4 and 5).

Table 3. Calculated ETCs. These ETCs are ordered from highest to lowest value. The higher value indicates greater QMIRW and lower QMCRW

No	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	E-	E+	EP	ETC	QMIRW	QMCRW
1	**Hexane*	*Hexane*	*-11.277*	*3.363*	*14.640*	*0.017*	*0.093*	*0.076*	*192.632*	*3.506*	*0.285*
2	Dichloromethane	Hexane	-10.582	3.363	13.945	-0.016	0.093	0.109	127.936	2.328	0.430
3	Hexane	Ethyl acetate	-11.277	1.052	12.329	0.017	0.119	0.102	120.873	2.200	0.455
4	Hexane	Ethanol	-11.277	3.334	14.611	0.017	0.151	0.134	109.037	1.984	0.504
5	Hexane	Dichloromethane	-11.277	0.521	11.798	0.017	0.130	0.113	104.407	1.900	0.526
6	Hexane	Methanol	-11.277	3.509	14.786	0.017	0.169	0.152	97.276	1.770	0.565
7	Dichloromethane	Ethyl acetate	-10.582	1.052	11.634	-0.016	0.119	0.135	86.178	1.568	0.638
8	Dichloromethane	Ethanol	-10.582	3.334	13.916	-0.016	0.151	0.167	83.329	1.516	0.659
9	Dichloromethane	Methanol	-10.582	3.509	14.091	-0.016	0.169	0.185	76.168	1.386	0.721
10	**Dichloromethane*	*Dichloromethane*	*-10.582*	*0.521*	*11.103*	*-0.016*	*0.130*	*0.146*	*76.048*	*1.384*	*0.723*
11	Methanol	Hexane	-11.139	3.363	14.502	-0.115	0.093	0.208	69.721	1.269	0.788
12	Ethyl acetate	Hexane	-11.250	3.363	14.613	-0.124	0.093	0.217	67.341	1.225	0.816
13	Ethanol	Hexane	-10.898	3.363	14.261	-0.119	0.093	0.212	67.269	1.224	0.817
14	Methanol	Ethanol	-11.139	3.334	14.473	-0.115	0.151	0.266	54.410	0.990	1.010

15	Ethyl acetate	Ethanol	-11.250	3.334	14.584	-0.124	0.151	0.275	53.033	0.965	1.036
16	*Ethanol	Ethanol	*-10.898*	*3.334*	*14.232*	*-0.119*	*0.151*	*0.270*	*52.711*	*0.959*	*1.042*
17	Methanol	Ethyl acetate	-11.139	1.052	12.191	-0.115	0.119	0.234	52.098	0.948	1.055
18	*Methanol	Methanol	*-11.139*	*3.509*	*14.648*	*-0.115*	*0.169*	*0.284*	*51.577*	*0.939*	*1.065*
19	*Ethyl acetate	Ethyl acetate	*-11.250*	*1.052*	*12.302*	*-0.124*	*0.119*	*0.243*	*50.626*	*0.921*	*1.085*
20	Ethyl acetate	Methanol	-11.250	3.509	14.759	-0.124	0.169	0.293	50.372	0.917	1.091
21	Ethanol	Ethyl acetate	-10.898	1.052	11.950	-0.119	0.119	0.238	50.210	0.914	1.094
22	Ethanol	Methanol	-10.898	3.509	14.407	-0.119	0.169	0.288	50.024	0.910	1.098
23	Methanol	Dichloromethane	-11.139	0.521	11.660	-0.115	0.130	0.245	47.592	0.866	1.155
24	Ethyl acetate	Dichloromethane	-11.250	0.521	11.771	-0.124	0.130	0.254	46.343	0.843	1.186
25	Ethanol	Dicholroetmethane	-10.898	0.521	11.419	-0.119	0.130	0.249	45.859	0.835	1.198

In this same table, columns 7, 8 and 9, 10 (relative values of the wells) can be seen that the cross-band interactions of the dichloromethane in both oxidizing-reductive directions are combined. The two cross-band interactions have different ETC values. In this case, dichloromethane is an oxidizing agent due to the lower value of its ETC (red letters).

The values of the ETCs of the upper phases are smaller, except the dichloromethane-ethyl acetate combination. If we place the larger masses at the bottom of the gravitational well, then the patterns are preserved, except the previous one (dichloromethane-ethyl acetate).

In figure 1, we can see that the dichloromethane-water combination has a different pattern. This pattern consists of two phases and an interface. The phase placed on the bottom is dichloromethane, the top phase is water.

Summing up all the previous observations, we can conclude that the gravitational well predominates the quantum well. It can infer that there are phases that have higher internal energy accumulated in the lower phases. The nature of this type of combinations can be explosive.

The differentiation of phases in the Dichloromethane-Water combination is due to the mass difference between the two combined substances (Table 4, sub-table D, column 8 and 10 and figure 2).

The difference between mass in the gravitational well of the Dichloromethane-Water mixture is 66.933 g/mol. The other mixtures of Dichloromethane the differences are smaller than this one. Due to these small differences, the other dichloromethane mixtures no interphase is observed, that it, the mixtures are homogeneous solutions.

In the diagram on the right of figure 2, it can be seen that both oxidations a reduction (crossed bands of the quantum well) are trapped at the interphase of the gravitational wells. It does no matter what the ETCs values of these crossed bands are different.

Table 4. Comparison of wells: Quantum vs. Gravitational.

A

						Relative difference		Relative ratio	
No.	**Oxidizin agent**	**Reducing agent**	**ETC**	**Mass**	**Location Phase**	**ETC**	**Mass**	**ETC**	**Mass**
10	*Dicholromethane	Dicholromethane	76.048	169.860	Upper	29.705	-3.180	1.641	0.982
7	Dicholromethane	Ethyl acetate	86.178	173.040	Intermediate	39.835	0.000	1.860	1.000
19	**Ethyl acetate**	**Dichloromethane**	**46.343**	**173.040**	**Intermediate**	**0.000**	**0.000**	**1.000**	**1.000**
24	*Ethyl acetate	Ethyl acetate	50.626	176.220	Lower	4.283	3.180	1.092	1.018

B

No.	**Oxidizin agent**	**Reducing agent**	**ETC**	**Mass**	**Location Phase**	**ETC**	**Mass**	**ETC**	**Mass**
9	*Methanol	Methanol	51.577	64.080	Upper	3.986	-52.890	1.084	0.548
10	Dicholromethane	Methanol	76.168	116.970	Intermediate	28.576	0.000	1.600	1.000
18	**Methanol**	**Dichloromethane**	**47.592**	**116.970**	**Intermediate**	0.000	0.000	1.000	1.000
23	*Dicholromethane	Dicholromethane	76.048	169.860	Lower	28.456	52.890	1.598	1.452

C

No.	**Oxidizin agent**	**Reducing agent**	**ETC**	**Mass**	**Location Phase**	**ETC**	**Mass**	**ETC**	**Mass**
16	*Ethanol	Ethanol	52.711	92.140	Arriba	6.852	-38.860	1.149	0.703
8	Dicholromethane	Ethanol	83.329	131.000	Interfase	37.470	0.000	1.817	1.000
25	**Ethanol**	**Dicholromethane**	**45.859**	**131.000**	**Interfase**	**0.000**	**0.000**	1.000	1.000
10	*Dicholromethane	Dicholromethane	76.048	169.860	Abajo	30.189	38.860	1.658	1.297

D

No.	**Oxidizin agent**	**Reducing agent**	**ETC**	**Mass**	**Location Phase**	**ETC**	**Mass**	**ETC**	**Mass**
1	*Water	Water	54.950	36.000	Upper	5.000	-66.933	1.100	0.350

2	Dicholro methane	Water	78.294	102.933	Intermediate	28.345	0.000	1.567	1.000
3	**Water**	**Dichloromethane**	**49.949**	**102.933**	**Intermediate**	0.000	0.000	1.000	1.000
4	*Dicholromethane	Dicholromethane	76.048	169.866	Lower	26.099	66.933	1.522	1.650

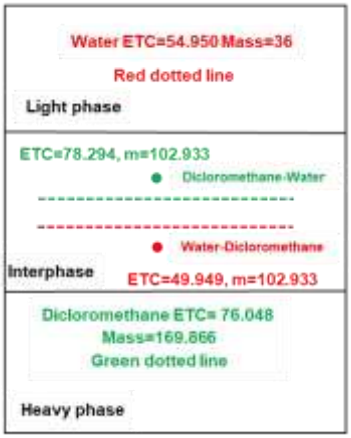

Figure 1. Dichloromethane-water (D). It can see the lower or heaver phase (dichloromethane), the interface and the upper face (water). Both oxidation an reduction area trapped at the interface due to the gravitational well (diagram on the right).

One hypothesis for new research is that:
"There is a turning point in the mass difference in the gravitational well that allows phase separation in a dichloromethane-X, where X is another substance."

If a study of limits and boundaries is made, the most stable mixture would be Heavy phase = higher molecular weight value and lower value of ETC. Interphase = Oxidation-Reducer with equal mass value and equal value of ETCs. Light or upper phase = Lower molecular weight value and lower value of ETC.

CONCLUSION

It was concluded: that ...

1. Hexane has the highest value of ETC. This means that hexane is the most unstable of the five solvents studied.
2. The Ethanol-Dichloromethane interaction has a smaller ETC of all. So this interaction is the most stable of all.
3. Three solvents were mixed, which yielded the last three interactions 23, 24 and 25 in the laboratory.
4. These three mixtures were utterly miscible. They formed single-phase solutions.
5. The water-dichloromethane mixture was made, and three phases were presented.
6. According to the quantum well and accurate gravitational calculations. The intermediate phase trapped the two quantum oxide-reduction wells, regardless of the value of each specific well.
7. With the ETC value of the quantum well of the water-dichloromethane mixture, it was determined that dichloromethane oxidize to water.
8. This finding explains that many substances with much internal energy are trapped in higher phases of a mixture. A mixture of this type can be eruptive.

REFERENCES

1. Caglieri, S. C., & Macaño, H. R. (2018). Reactividad de aminas en la acetilación catalizada por ácidos de Lewis e influencia de solventes: estudio teórico. Ingeniería, investigación y tecnología, 19(2), 239-244.
2. Sierra, J. J. B. (2018). Extração de lipídios da microalga Scenedesmus sp. Com diferentes mistura de solventes orgânicos. Biotecnología en el Sector Agropecuario y Agroindustrial, 16(2), 88-98.
3. Ramos, I. T., da Silva, T. M., Silva, T., & Camara, C. A. (2018). Environmental friendly methods for regioselective iodination of the 3, 7, 3', 4'-tetramethoxy-quercetin. Química Nova, 41(5), 577-580.
4. Becerra, R., Conde, J., Cardona, Y., & Torres, A. (2018). Cuantificación del flavonoide quercetina en miel de Apis mellifera, mediante DMFS–UV-Vis. Semilleros de investigación, 1(1).
5. Ramírez-Rojo, M. I., Vargas-Sánchez, R. D., del Mar Torres-Martínez, B., Torrescano-Urrutia, G. R., & Sánchez-Escalante, A. (2018). Extractos de hojas de plantas para conservar la calidad de la carne y los productos cárnicos frescos. Revisión. Biotecnia, 20(3), 155-164.
6. Baños, S. B., Necha, L. L. B., Lauzardo, A. N. H., Velázquez-del Valle, M., Tejacal, I. A., & Sánchez, D. G. (2018). Polvos, extractos y fracciones de hojas de Cestrum nocturnum L. y su actividad antifúngica en dos aislamientos de Fusarium spp.| Powders, extracts and fractions of leaves of Cestrum nocturnum L. and their antifungal activity over two isolations of Fusarium spp. UDO Agrícola, 8(1).
7. Sinisterra, A. F. V., Vidal, A. P., & Orrego, A. R. (2018). Evaluación in vitro de la actividad antiplasmodial y citotóxica de plantas del sur pacífico colombiano (Tumaco, Nariño). Biotecnología en el Sector Agropecuario y Agroindustrial, 16(2), 79-87.
8. Arguedas, M., Hilje, L., Cartín, V., Calvo, M. A., & Borbón, H. (2018). Phagodeterrence of extracts ofBrugmansia candida (Solanaceae) onHypsipyla grandella (Lepidoptera: Pyralidae) larvae. Revista de Biología Tropical, 66(1), 58-69.
9. Parra, M. G., Lizama, R. S., & Fidalgo, L. M. (2018). Estudio antileishmanial y citotóxico bio-guiado de fracciones y sub-fracciones de Bio-guide antileishmanial and cytotoxic study of fractions and sub-fractions from Pluchea carolinensis (Jacq.) G. Don (Asteraceae). Revista Cubana de Farmacia, 51(2).
10. Ettiene, G., Montero, P. G., Bauza, R., Sandoval, L., & Medina, D. (2018). Persistencia del insecticida Clorpyrifos en hojas y tallos de guayabo (Psidium guajava L.)| Persistence of Chlorpyrifos pesticide in leaves and stems of guava-tree (Psidium guajava L.). UDO Agrícola, 10(1).
11. Capuñay Reyes, P. P. (2018). Sistemas de extracción de biomoléculas con actividad antibiótica de Rapidithrix sp. de playa Laguna Grande-Paracas. Universidad Nacional de Trujillo. Tesis. Repositorio.
12. Castro, O., Gutiérrez, J. M., Barrios, M., Castro, I., Romero, M., & Umaña, E. (1999). Neutralización del efecto hemorrágico inducido por veneno de Bothrops asper (Serpentes: Viperidae) por extractos de plantas tropicales. Revista de Biología Tropical, 47(3), 605-616.
13. Pineda, M. E., & Rodríguez-Acosta, A. (2018). El impresionante universo de los venenos, su variabilidad bioquímica, hemostática y tóxica en las serpientes (Serpentes: Viperidae) Porthidium y Bothrops| The impressive universe of the venoms, their biochemical, haemostatic and toxic variability in Porthidium and Bothrops (Serpentes: Viperidae) snakes. SABER, 30, 265-283.
14. Martínez, D., Chávez, M., Díaz, A., Chacín, E., & Fernández, N. (2003). Eficiencia del Cactus lefaria para su uso como coagulante en la clarificación de aguas. Revista Técnica de la facultad de ingeniería Universidad del Zulia, 26(1), 27-33.
15. González-Pérez, M. (2017). Quantum Theory of the Electron Transfer Coefficient. International Journal of Advanced Engineering, Management and Science, 3(10).
16. González-Pérez, M., Gonzalez-Martinez, D., González-Martínez, E. L., Pacheco-Bautista, D., & Medel-Rojas, A. (2018). Theoretical-Chemical-Quantum Analisys of Sarin Neurotoxicity. World Journal of Pharmacy and Pharmaceutical Sciences, 7(5), 173-180.
17. García-Aguilar, K., Herrera-Cantú, I., Pedraza-Gress, E., Flores-Gonzalez, L. A., Aparicio-Razo, M., Sánchez-Parada, O., ... & González-Pérez, M. Quantic Analysis of Formation of a Biomaterial of Latex, Retinol, and Chitosan for Biomedical Applications. International Journal of Advanced Engineering, Management and Science, 4(1).
18. Herrera-Cantú, I., García-Aguilar, K., Pedraza-Gress, E., Vázquez, E., García-Mar, J. J., Flores-González, L. A., ... & González-Pérez, M. Quantic Analysis of the Adherence of a Gram-Negative

Bacteria in A HEPA Filter. International Journal of Advanced Engineering, Management and Science, 3(12).
19. González-Pérez, M. (2017). Chemical-quantum Analysis of the Aggressiveness of Glucose and its Appeasement with ATP Inside the Cell, and Water as an Excellent Antioxidant. World Journal of Pharmacy and Pharmaceutical Sciences, 6(4), 95-99.
20. Pacheco-García, P. F., Perez-Gonzalez, A., Ramos-Flores, A., Flores-Gonzalez, L. A., Lopez-Oglesby, J. M., & Gonzalez-Perez, M. Experimental study and calculation of the electron transfer coefficients on the dissolution behavior of chitosan in organic acids. International Journal of Advanced Engineering, Management and Science, 3(6).
21. González-Perez, M. (2017). Interactions analysis of four chemotherapeutic drugs vs. nitrogenous bases of DNA and RNA, using quantum methods. World Journal of Pharmaceutical Research, 5(6), 309-320.