THEORETICAL CALCULATION OF ELECTRON TRANSFER COEFFICIENT FOR PREDICTING THE FLOW OF ELECTRONS BY PM3, USING 20 AMINO ACIDS AND NICOTINE

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Abstract

In this work, an Electron Transfer Coefficient (ETC) it derived for various chemical species to help predict the flow of electrons in amino acid-nicotine interactions. The quantum method "Semi-Empirical Parameterized Models Number 3" (SE-PM3) was set to calculate the variables HOMO-LUMO, the Gap Band (BG) and the Electrostatic Potential (EP) of 20 Amino Acids (AA) and Nicotine. In conclusion, the electrons need more energy to jump their BG when the ETC is large; thus, the electrons flow toward the lower value of the ETC. Tryptophan has an ETC = 19.1, Isoleucine has an ETC = 54.573, and Nicotine has an ETC = 40.873. The ETC of nicotine is in the middle of the ETC of 20 different AA.

Keywords: Electron Transfer Coefficient, Quantum Method PM3; HOMO-LUMO; Band Gap; Electrostatic Potential

Introduction

Electron transfer is an area widely studied in many fields of science. By examples: the chemistry of ceramics in which the consumption of ions is favored by decreasing the difference in Fermi energies (Fernández-Ibañez, 2000). The photochemical decarboxylation of carboxylic acids in organic chemistry (Yoshimi, 2010) and nanocomposites of fullerenes (Ito, 2012),

functionalized anthraquinone (Bezaine, 2005). The photo-induced electron transfers on a donor-acceptor system for converting solar energy into electrical power (Langa, 2012). Because of these fields of study, researchers have achieved the construction of optoelectronic devices (Kadish, 2010) and, it developed processes that are more efficient.

In biochemistry, electron transfer generates reactions essential for life (Van der Ham, 2014). In the emerging field of the metalloprotein designs, researchers seek to prepare artificial proteins whose properties can mimic and perhaps improve many features found in natural metalloenzymes (Ogawa, 2006). Investigators have studied nicotine in its interactions with living matter extensively. An interesting study is the formation of carcinogens indoors, and its dangers from second and third-hand smoke (Sleimana, 2010).

Quantum chemistry is a useful tool in these endeavors and has an important role in describing electron transfer. Relatively simple methods, such as SE-PM3 are available for calculating the nuclear reorganization of energy matrix elements and electronic coupling (Amini, 2003). There are different ways and methods to estimate the same parameter or variable. As an example, the variables and parameters of compounds used to treat Parkinson's disease, such as 4-acetylamino-2- (3, 5-dimethyl pyrazol-1-y l)-6-pyridyl pyrimidine were calculated successfully (Morales-Bayuelo, 2014). Quantum methods allow the detection of various molecular structures before undertaking a synthetic extensive program (Greerling, 2002), (Abdallah, 2012).

In this work, it proposed and derived using computational quantum chemistry methods an ETC to predict the flow of electrons in a given chemical system. As a test case, it calculated the coefficients for 20 AA and nicotine by the SE-PM3 method to organize the flow of electrons, predict chemical reactions, or transfer electrons from a molecule to molecule.

Materials and methods

It bought the molecular simulator Hyper Chem (HC). (Hyper Chem. Hypercube, MultiON for Windows. Serial #12-800-1501800080. MultiON. Insurgentes Sur 1236 - 301 Tlacoquemecatl Col. del Valle, Delegación Benito Juárez, D. F., México CP. 03200.)

It used HC SE-PM3 to draw the corresponding molecules. Then it selected, SE-PM3. It optimized the geometry with the Polak Ribiere method and conducted the calculation of the variables of HOMO-LUMO, BG, EP and other properties, resulting in a Tab-delimited table for BG and EP for AA.

The specific parameters selected for each of the simulations were as follows:

SEMIEMPIRICAL PM3

Total Charge 0. Spin Multiplicity1. Spin Pairing RHF. State Lowest Converget Limit 0.01. Interation Limit 50. Accelerate Convergence Yes. Polarizibility Not. Geometry Optimization: Algoritm Polak-Ribiere (Conjugate gradient). Termination condition RMS gradient of 0.1 kcal/Amol. Algoritm Polak-Ribiere (Conjugate gradient), Termination condition or 255 maximun cycles. Algoritm Polak-Ribiere (Conjugate gradient) Termination condition or In vacuo. Screen refresh period 1 cyclest.

PLOT OF ELECTROSTATIC POTENTIAL

Molecular Property: Property Electrostatic Potential, Representation 3D. Mapped Isosurface. Isosufrace Grid: Grid Mesh Size Fine. Isosufrace Grid: Grid Layout Defoult. Contour Grid Starting Value Defoult. Contour Grid Increment 0.05. Mapped Funtion Options Defoult. Transparency Level a criteria. Isosurface Rendering. Total charge density 0.01. Rendering Wire mesh.

FORMULATION

BG was calculated by the formula BG = $\left|\text{HOMO-LUMO}\right|$ (Odunola, 2007) and EP from the formula EP = $\left|\text{E+ - E-}\right|$. The ETC it calculated as enunciated in equation 1.

HARDWARE

Microsoft. Hardware ATA ST500DM002 IDB14SCSI. 6.1.7600.16385.

Result and discussion

Table 1 shows the BG values calculated in eV from lowest to highest in the fourth column. It observed that the Serine has the largest amount of BG. In contrast, Tryptophan has the lowest value of BG; thus, the valence electrons of tryptophan cross the smaller BG while the Serine electrons must pass a larger BG.

Table 1 Values of BG of 20 AA in eV

No.	AA	HOMO	LUMO	BG
1	Tryptophan	-6.553	-2.141	4.412
2	**Nicotine**	**-9.065**	**-0.154**	**8.910**
3	Methionine	-9.100	0.106	9.206
4	Tyrosine	-9.398	-0.113	9.284
5	Cysteine	-9.287	0.077	9.364
6	Phenylalanine	-9.503	0.248	9.751
7	Histidine	-9.455	0.524	9.979
8	Arginine	-9.374	0.821	10.195
9	Threonine	-10.003	0.468	10.471
10	Aspartic acid	-10.129	0.399	10.527
11	Glycine	-9.521	1.035	10.556
12	Lysine	-9.521	1.035	10.556
13	Prolyne	-9.617	1.066	10.683
14	Leucine	-9.884	0.867	10.751

15	Glutamic acid	-10.079	0.675	10.754
16	Glutamine	-10.019	0.736	10.756
17	Valine	-9.829	0.937	10.766
18	Asparagine	-10.197	0.577	10.774
19	Alanine	-9.925	0.936	10.861
20	Isoleucine	-10.112	1.075	11.188
21	Serine	-10.483	0.876	11.360

Given the same electrostatic potential for these listed AA, then the Tryptophan electrons need fewer times their electrostatic potential to cross the BP.

By its nature, the EP varies in each AA, as shown in Table 2. Here, it was necessary to create an ETC to compare and quantify the flow direction of electron in chemical species.

Table 2.Values of EP of 20 AA and Nicotine (eV)

No.	**AA**	**E+**	**E-**	**EP**
1	Leucine	0.094	-0.11	0.204
2	Isoleucine	0.123	-0.082	0.205
3	Valine	0.132	-0.08	0.212
4	**Nicotine**	**0.09**	**-0.128**	**0.218**
5	Tryptophan	0.09	-0.141	0.231
6	Glycine	0.1	-0.131	0.231
7	Phenylalanine	0.113	-0.119	0.232
8	Lysine	0.132	-0.101	0.233
9	Serine	0.107	-0.134	0.241
10	Alanine	0.114	-0.128	0.242
11	Cysteine	0.126	-0.12	0.246
12	Threonine	0.143	-0.114	0.257
13	Asparagine	0.133	-0.127	0.26
14	Methionine	0.137	-0.123	0.26
15	Glutamic acid	0.137	-0.125	0.262
16	Proline	0.13	-0.134	0.264
17	Glutamine	0.135	-0.134	0.269
18	Aspartic acid	0.146	-0.127	0.273
19	Arginine	0.135	-0.139	0.274
20	Tyrosine	0.152	-0.134	0.286
21	Histidine	0.14	-0.161	0.301

Table 2 shows EP values, lowest to highest in the fourth column. It observed that Histidine has the highest value of EP, whereas Leucine has the lowest value. It interpreted that the valence Histidine electrons have more energy available to cross its BG than Leucine electrons. With these two variables calculated for the chemical species in question, it is possible postulate a definition for the ETC:

Equation 1

ETC = BG/EP

The ETC between molecules is equal to the division of the value of the BG (Table 1) by the value of EP (Table 2). The calculated ETC values it found in Table 3.

Table 3 Values of ETC of 20 AA and Nicotine

No.	AA	ETC
1	Tryptophan	19.100
2	Tyrosine	32.463
3	Histidine	33.153
4	Methionine	35.407
5	Arginine	37.209
6	Cysteine	38.067
7	Aspartic acid	38.561
8	Glutamine	39.984
9	Proline	40.466
10	Threonine	40.742
11	**Nicotine**	**40.873**
12	Glutamic acid	41.045
13	Asparagine	41.438
14	Phenylalanine	42.030
15	Alanine	44.879
16	Lysine	45.304
17	Glycine	45.696
18	Serine	47.135
19	Valine	50.783
20	Leucine	52.702
21	Isoleucine	54.573

Interpretation of etc

Higher values of ETC indicates that electrons have greater difficulty in passing from molecule to molecule of the same chemical species (which is similar to the electronic impedance), and lower values of ETC indicate easier electron transfer.

The ETC is the multiple of its EP a chemical species needs to hop through its BG. In the particular case of ETC values of the studied AA, tryptophan needs 9.1 times its EP for its valence electrons to jump to a neighboring molecule of the same species. In the case of cysteine, whose ETC is 54.573, it would interpret this as meaning it requires 54.573 times its PE to transfer its electrons to the same system.

Nicotine

With the same methodology, the ETC of nicotine it calculated as 40.873, placing it in the middle of all AA values. Given identical conditions for AA and nicotine, the electrons of nicotine have similar difficulties to jump its BG because nicotine is reactive or transfers its electrons with 20 AA.

The cross bands of nicotine with two AA tryptophan and isoleucine it calculated, with the results shown in Table 4 for the nicotine-tryptophan interaction and Table 5 for the nicotine-isoleucine interaction.

Where:

NE+, NE-, TE+, TE-, IE+, IE- are the particular EPs of Nicotine, Tryptophan, and Isoleucine, respectively, and NL, NH, TL, TH, IL, IH, is HOMO-LUMO of Nicotine, Tryptophan, and Isoleucine, respectively.

Table 4 Cross-Band of Nicotine vs Tryptophan

Cross	EP	Cross	BG	ETC
NE+ vs NE-	0.218	NL vs NH	8.910	40.873
NE+ vs TE-	0.231	NL vs TH	6.399	27.701
TE+ vs TE-	0.231	TL vs TH	4.412	19.100
TE+ vs NE-	0.218	TL vs NH	6.923	31.759

Table 5 Cross-Band or Nicotine vs Isoleucine

Cross	EP	Cross	BG	ETC
N+ vs N-	0.218	NL vs NH	8.910	40.873
N+ vs I-	0.172	NL vs IH	9.958	57.896
I+ vs I-	0.205	IL vs IH	11.188	54.573
I+ vs N-	0.251	IL vs NH	10.140	40.397

The most probable direction of the electrons at the first intersection is TH to TL (Fig. 1) due to the lower value of the ETC, while for the second crossing it is NH to IL (Fig 2). In the first case, there is a very low probability that nicotine reacts with tryptophan. The second case is very likely that nicotine reacts with isoleucine.

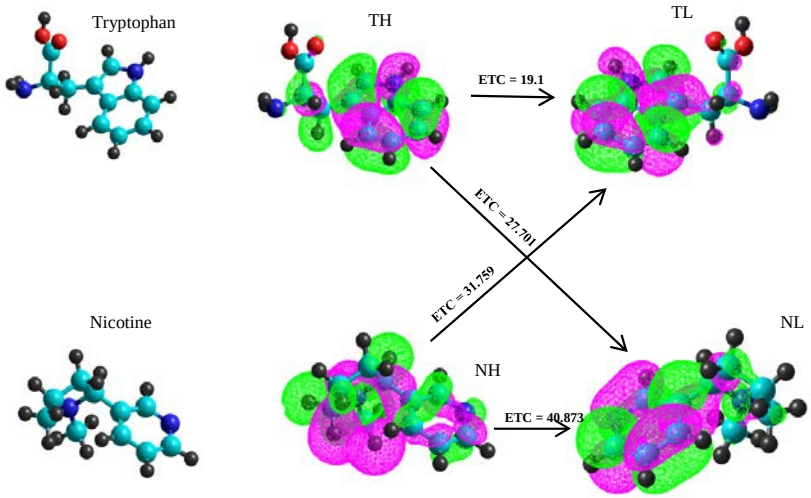

Figure 1 Cross-band Tryptophan vs. Nicotine

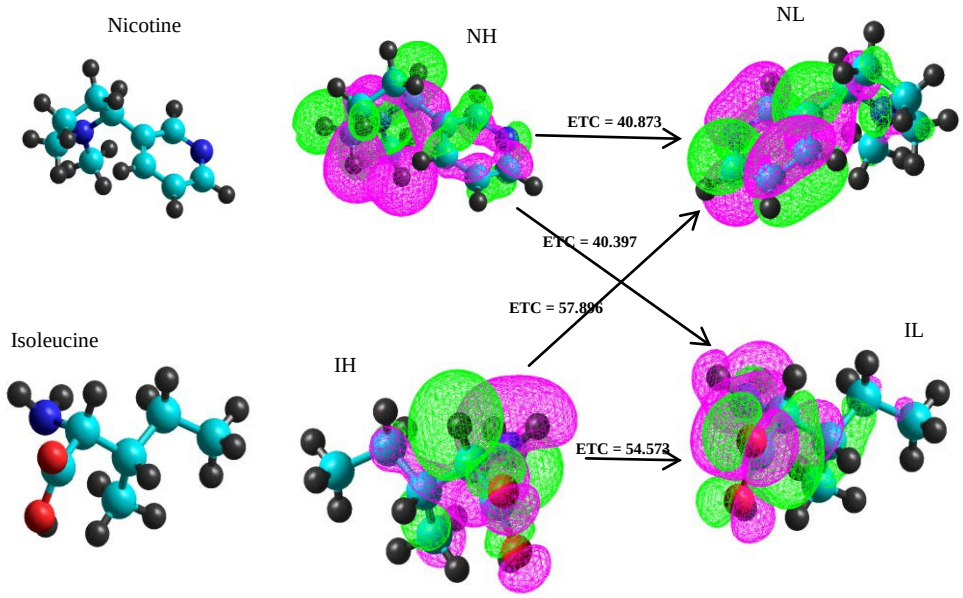

Figure 2 Cross-band Isoleucine vs. Nicotine

Conclusion

The electrons can jump a BG where its ETC has a lower value. If the ETC is lower in the same species, then the electrons jump the BG more quickly. Because of this, the substance is more likely to be stable and has a lower probability of reactivity. In the test cases, tryptophan has an ETC = 19.1, isoleucine has an ETC = 54.573, and nicotine has an ETC = 40.873. The ETC for nicotine is in the center of the 20 AA ETCs. In the example: nicotine (40.873) vs. tryptophan (19.1) and nicotine vs. Isoleucine (54.573), nicotine would react with Isoleucine, but probably not with tryptophan.

In general, when the internal ETC is highest (including cross-band ETCs) the probability of a chemical reaction is high. In other words, the valence electrons will move where the ETC has the smallest value.

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