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ANALYSIS OF NITROGEN BASES ALTERATIONS IN DNA AND RNA CAUSED BY AIR POLLUTANTS BY QUANTUM METHODS

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ABSTRACT

Currently, air pollution is a worldwide problem, where the main air pollutants are sulfur dioxide (SO2), nitrogen oxides (NxOx), carbon oxides (COx), particulate matter (PM), ozone (O3) and Pb due its high concentration and impact they cause. The relation of the bases is the key, and the structure of DNA has important implications, allowing processes such as DNA replication and RNA translation into protein. The formation of protein-nucleic acid associations proceeds through hydrogen bonds. The simulations realized with molecular simulator Hyper Chem (HC). We performed electronic interactions between molecules of the same, the interactions of cross-bands of the nitrogenous bases and the interactions of cross-bands of air pollutants. From these simulations we infer as the principal contribution of this study, that C can be confused with the N_2O_3, G can be confused with SO_2; CO_2; CO; O_3 and with the Pb in the genesis of RNA. Because the similar value of ETC of C:G. With these findings, another avenue to explain the oncogenic and mutagenic effects of N_2O_3, SO_2, CO_2, CO, O_3 and the Pb on the human body are proposed in conjunction with the novel ETC method.

KEYWORDS: Air pollutants, Nitrogenous bases, Cancer, Quantum Methods.

INTRODUCTION

a. Air pollutants

Currently, air pollution is a worldwide problem, caused by a lot of amount of pollutants emitted by fossil combustion processes, from the chemical industry, thermoelectric [1], and overexploitation of natural resources. The main air pollutants are sulfur dioxide (SO_2), nitrogen oxides (NxOx), carbon oxides (COx), particulate matter (PM), ozone (O_3) and Pb [2-5] due its high concentration and impact they cause. In investigations, it has shown that air pollutants cause diseases respiratory, diseases skin diseases cardiovascular [6-11]. Fine particles and sulfur dioxide increase the risk of heart disease among people of low social class especially African Americans [12]. The main air pollutants that cause effects in the skin are solar UV, HAP, VOC, NOx, PM, O_3, radiation and cigarette smoke can contribute to skin aging, atopic dermatitis, skin cancer, psoriasis and acne [13]. Epidemiological studies show that long-term exposure to particulate matter is related to an increased risk of cancer [14]. Research conducted they found evidence that exposure to fine particles has a significant increase in mortality from lung cancer, even after controlling for smoking, occupational exposure, and other risk factors [15].

b. Nitrogenous bases

The form double helical from DNA in its more common forms gives stability to preserve the genetic information of this vital molecule of Life [16-17].

Nitrogenous bases are those that contain genetic information. In the case of DNA, are bases purines and pyrimidines. Purines are adenine (A) and guanine(G). Pyrimidines are thymine (T) and cytosine (C). In the case of RNA are also four bases, two purines, and two pyrimidines. Purines are A and G and pyrimidines are cytosine (C) and uracil (U).

The nitrogenous bases are complementary to each other, form pairs just as they would a key and a lock. Adenine and thymine are complementary (A-T), as guanine and cytosine (G-C), in the RNA is not exists the thymine, complementarity is between adenine and uracil (A-U). The relation of the bases is the key, and the structure of DNA has important implications, allowing processes such as DNA replication and RNA translation into protein. The formation of protein-nucleic acid associations proceeds through hydrogen bonds [18].

c. Quantum computational methodology

Quantum chemistry it is a science that expresses the fundamental behavior of matter at the molecular scale mathematically [19]. Quantum chemistry has several uses one of them is the study of the behavior of atoms and molecules in their optical, electrical, magnetic, mechanical properties, chemical reactivity, its redox properties, and so on. Friedrich Hund and Robert S. Mulliken developed the molecular orbital theory, an alternative method in where described the electrons by mathematical functions delocalized throughout the molecule. The method Hund-Mulliken (or molecular orbital) virtually, is the most widely used in recent years as the most powerful predictor properties. Computational quantum chemistry-based methods identify identity also more stable molecular systems which tautomers for the common chemical knowledge is not enough to make definitive predictions[20].

Computational methods are imperative in predicting chemical and biochemical reactions. These methods can save time, materials and reagents in laboratory experiments[21].

For this work, we explored the molecular interactions of air pollutions and the nitrogenous bases of DNA and RNA by the quantum method SE-PM3.

II. METHODOLOGY

a. Abbreviations

Occupied Molecular Orbital higher (HOMO). Molecular lowest unoccupied orbital (LUMO). Band Gap (BG). Negative energy (E). Positive energy (E+). Electrostatic potential (EP). Electronic transfer coefficient (ETC).

b. Computational methods

The simulations realized with 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) [22].

The computational model used was; HC Semi-Empirical Parameterized Model number 3 (SE- PM3) to draw the corresponding molecules. These were then processed using SE-PM3 The geometry realized with the Polak Ribiere method.

We calculate the computational quantum chemistry variables: HOMO-LUMO, BG, EP and other properties, resulting in a Tab-delimited Table for BG and EP.

The specific parameters selected for each of the simulations were as follows: SET UP. Semi-Empirical Method: PM3. Semi-Empirical Options: Charge and Spin. Total Charge 0. Spin Multiplicity 1. SCF Control. Converge limit 0.01. Interaction limit 1000. Accelerate converge Yes. Spin Pairing Lowest. Overlap Weighting Factors Sigma-Sigma 1, Pi-Pi 1. Polarizabilities do not calculate.

Computation 1. Geometry Optimization. Algorithm Polak Ribiere (conjugate gradient). Options Termination conditions. RMS gradient of 0.1 kcal/mol or 1000 maximum cycles. In vacuo yes. Screen refresh period one cycles [22].

Computation 2. Orbitals. Plot Orbital Options Isosurface Rendering. Orbital Contour Value 0.05. Rendering Wire meshes Isosurface Grid. Grid meshes size Coarse. Grid layout Default. Gird contour Default. Transparency level Default [22].

Computation 3. Plot Molecular Graphs. Plot Molecular Options. Molecular Properties. Properties. Electrostatic Potential Yes. Representations. 3D Mapped Isosurface. Grid Mesh Size Coarse. Grid layout Default. Contour gird Default. Isosurface Rereading. Total Charge Density Contour Value (TCDCV) 0.015. Rendering Wire mesh [22]. Transparency level Default. Mapped Options Functions Default.

c. Formulas

The calculations based on the theory of ETC [23]. This theory is calculating the ratio of dividing the BG / EP. This ratio Indicates the multiples of the EP ITS That the electron jumps BG [19].

$$ETC = \left|\frac{BG}{EP}\right| \quad (1)$$

The EP is equal to the absolute value of the difference (E+) – (E-).

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

The BG is equal to the absolute value of the difference (HOMO) – (LUMO) [22-24].

$$BG = |HOMO - LUMO| \quad (3)$$

III. RESULT AND DISCUSSION

Table 1 shows the results obtained. We performed electronic interactions between molecules of the same column sorted by ETC; this order indicates the stability of substances. The interplay 1 (G:G) is the most stable, and interaction 12 (Pb) is the least stable. The most unstable molecule is the O_3.

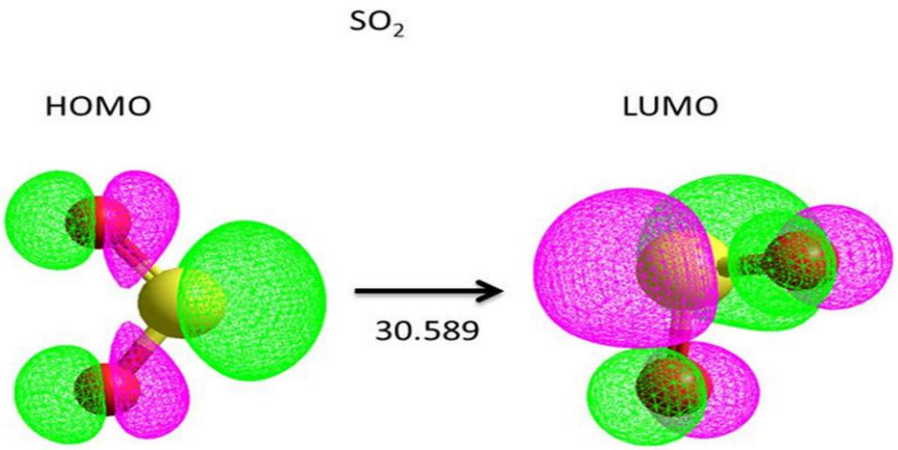

Fig. 1 interaction between two molecules of Sulfur dioxide

Table 1. Electronic interactions between molecules of the same chemical species.

Interaction number	Gives electron cloud	Get electron cloud	HOMO (eV)	LUMO (eV)	BG (eV)	E- (eV/a0)	E+ (eV/a0)	EP (eV/a0)	ETC*
1	G	G	-8.537	-0.206	8.331	-0.150	0.172	0.322	25.872
2	C	C	-9.142	-0.344	8.799	-0.174	0.161	0.335	26.265
3	U2	U2	-9.910	-0.415	9.495	-0.147	0.202	0.349	27.208
4	A	A	-8.654	-0.213	8.441	-0.140	0.156	0.296	28.518
5	SO2	SO2	-10.551	1.530	12.082	-0.147	0.248	0.395	30.589
6	T	T	-9.441	-0.475	8.966	-0.123	0.169	0.292	30.707
7	U1	U1	-9.710	-0.511	9.200	-0.126	0.171	0.297	30.975
8	N_2O_3	N_2O_3	-11.108	-0.799	10.309	-0.051	0.188	0.239	43.135
9	CO_2	CO_2	-12.735	1.036	13.772	-0.072	0.164	0.236	58.356
10	CO	CO	-13.027	1.000	14.027	-0.057	0.131	0.188	74.616
11	O_3	O_3	-13.007	-0.616	12.391	-0.034	0.075	0.109	113.682
12	Pb	Pb	-18.626	5.087	23.713	0.020	0.022	0.002	11856.55

*The ETC is considered dimensionless. Energy unit is the electron volt (eV).

The unit of Electrostatic Potential is (electron - volt) / Angstroms.

The reactivity behaves in the opposite direction. From the least to ETC = 113.682 are the highest among all substances in Table 1. This interaction 11 belongs to the molecule of O_3 Therefore; the order of the ETCs indicates that the Pb, O_3, CO, N_2O_3 attacks anyone of nitrogenous bases.

Table 2 shows the interactions of cross-bands of the nitrogenous bases. We tabulated by the ETC values (last column). It was according to the Lane prediction [25].

The lower ETC = 23.074 belong to the interaction G:U2. This interaction is a mispair occurring DNA or RNA. G:U1 or G:U2. The glycosylase removed mispairs from DNA by uracil-DNA (UDG) [26-28] UDG is highly specific for U and shows no activity towards any other base. Specifics for U and shows no activity towards any other based [28-29].

In general, the base pair partner of the U is not recognized, and the enzyme also acts on A:U base pairs that arise through misincorporation during DNA replication [29-30].

Furthermore, we can speculate that the small differences between the bases ETCs indicate that the probability of unwanted combined pairs of both DNA and RNA are high. Therefore, mutations are very likely in different directions of flow of electrons [23].

Table 2. Electronic interactions between molecules nitrogenized bases. Cross band.

Interaction number	Gives electron cloud*	Get electron cloud**	HOMO	LUMO	BG	E-	E+	EP	ETC
1	G	U2	-8.537	-0.415	8.122	-0.150	0.202	0.352	23.074
2	C	U2	-9.142	-0.415	8.728	-0.174	0.202	0.376	23.212
3	A	U2	-8.654	-0.415	8.240	-0.140	0.202	0.342	24.092
4	G	U1	-8.537	-0.511	8.026	-0.150	0.171	0.321	25.003
5	C	U1	-9.142	-0.511	8.632	-0.174	0.171	0.345	25.019
6	C	T	-9.142	-0.475	8.668	-0.174	0.169	0.343	25.270
7	G	T	-8.537	-0.475	8.062	-0.150	0.169	0.319	25.273
8	C	G	-9.142	-0.206	8.936	-0.174	0.172	0.346	25.827
9	G	G	-8.537	-0.206	8.331	-0.150	0.172	0.322	25.872
10	A	U1	-8.654	-0.511	8.144	-0.140	0.171	0.311	26.185
11	C	C	-9.142	-0.344	8.799	-0.174	0.161	0.335	26.265
12	G	C	-8.537	-0.344	8.193	-0.150	0.161	0.311	26.345
13	A	T	-8.654	-0.475	8.180	-0.140	0.169	0.309	26.471
14	C	A	-9.142	-0.213	8.929	-0.174	0.156	0.330	27.058
15	A	G	-8.654	-0.206	8.448	-0.140	0.172	0.312	27.078
16	G	A	-8.537	-0.213	8.324	-0.150	0.156	0.306	27.202
17	U2	U2	-9.910	-0.415	9.495	-0.147	0.202	0.349	27.208
18	A	C	-8.654	-0.344	8.311	-0.140	0.161	0.301	27.610
19	T	U2	-9.441	-0.415	9.026	-0.123	0.202	0.325	27.773
20	U1	U2	-9.710	-0.415	9.296	-0.126	0.202	0.328	28.340
21	A	A	-8.654	-0.213	8.441	-0.140	0.156	0.296	28.518
22	U2	U1	-9.910	-0.511	9.399	-0.147	0.171	0.318	29.558
23	U2	T	-9.910	-0.475	9.435	-0.147	0.169	0.316	29.859

24	T	U1	-9.441	-0.511	8.930	-0.123	0.171	0.294	30.375
25	U2	G	-9.910	-0.206	9.704	-0.147	0.172	0.319	30.420
26	T	T	-9.441	-0.475	8.966	-0.123	0.169	0.292	30.707
27	U1	U1	-9.710	-0.511	9.200	-0.126	0.171	0.297	30.975
28	U2	C	-9.910	-0.344	9.567	-0.147	0.161	0.308	31.061
29	T	G	-9.441	-0.206	9.235	-0.123	0.172	0.295	31.305
30	U1	T	-9.710	-0.475	9.236	-0.126	0.169	0.295	31.307
31	U1	G	-9.710	-0.206	9.504	-0.126	0.172	0.298	31.894
32	U2	A	-9.910	-0.213	9.697	-0.147	0.156	0.303	32.004
33	T	C	-9.441	-0.344	9.098	-0.123	0.161	0.284	32.033
34	U1	C	-9.710	-0.344	9.367	-0.126	0.161	0.287	32.637
35	T	A	-9.441	-0.213	9.228	-0.123	0.156	0.279	33.076
36	U1	A	-9.710	-0.213	9.497	-0.126	0.156	0.282	33.679

*These substances are reducing agents because they are oxidized.

**These substances are oxidizing agents because they are reduced.

Table 3 shows the possible "allowed interactions" between the nitrogenous bases in DNA and RNA. The difference between ETCs interactions cross bands is minimum. This affirmation leads us to say that any of them occurs easily and reaffirms the formation of hydrogen bond of low energy.

The ETC = 24.092 corresponding to the interaction A:U2 is the lowest of the table. This lowest ETC means that is the most likely to occur under these conditions.

Table 3. Possibles pairs interactions between the nitrogenous bases in DNA and RNA.

Interaction number	Gives electron cloud	Get electron cloud	HOMO	LUMO	BG	E-	E+	EP	ETC
3	A	U2	-8.654	-0.415	8.240	-0.140	0.202	0.342	24.092
8	C	G	-9.142	-0.206	8.936	-0.174	0.172	0.346	25.827
10	A	U1	-8.654	-0.511	8.144	-0.140	0.171	0.311	26.185
12	G	C	-8.537	-0.344	8.193	-0.150	0.161	0.311	26.345
13	A	T	-8.654	-0.475	8.180	-0.140	0.169	0.309	26.471
32	U2	A	-9.910	-0.213	9.697	-0.147	0.156	0.303	32.004
35	T	A	-9.441	-0.213	9.228	-0.123	0.156	0.279	33.076
36	U1	A	-9.710	-0.213	9.497	-0.126	0.156	0.282	33.679

This table is a part of Table 2.

Table 4 shows the lowest energy interactions of the four hydrogen bonds of the nitrogenous bases in DNA and RNA. The divergence between the highest and the lowest value for the ETCs in Table 4 is 2.38; The interactions 3, 10 and 13 show the best affinity of the A for the U2 and U1 than the T.

Table 4. The lowest energy interactions of the four hydrogen bonds of the nitrogenous bases in DNA and RNA.

Interaction number	Gives electron cloud	Get electron cloud	HOMO	LUMO	BG	E-	E+	EP	ETC
3**	A	U2	-8.654	-0.415	8.240	-0.140	0.202	0.342	24.092
8*	C	G	-9.142	-0.206	8.936	-0.174	0.172	0.346	25.827
10*	A	U1	-8.654	-0.511	8.144	-0.140	0.171	0.311	26.185
13**	A	T	-8.654	-0.475	8.180	-0.140	0.169	0.309	26.471

This table is a part of Table 3.

* The Interactions of lower energy (more stable) for the DNA.

* *The Interactions of less energy (more stable) for the RNA.

The next tables show the interactions between the principal air pollutants with nitrogenous bases in crossbands.

Table 5 lists the interactions between N_2O_3 with nitrogenous bases in crossbands. The ETC = 24.092 (Table 4 A:U2) and ETC = 22.892 of (Table 5 G:N_2O_3) are nearly equal. This comparison indicates that the N_2O_3 competes with A by U2. This competition allows N_2O_3 can be confused with the A. The probability of that this confusion causes a mutation, is very high.

The ETC = 26.471, (Table 4 A:T) and ETC = 27.195 (Table 5 U2: N_2O_3) are similar and can also cause confusion.

Table 5. Interactions between N_2O_3 with nitrogenous bases in cross bands.

Interaction number	Gives lectron cloud	Get lectron cloud	HOMO	LUMO	BG	E-	E+	EP	ETC
1	G	N_2O_3	-8.537	-0.800	7.737	-0.150	0.188	0.338	22.892
2	C	N_2O_3	-9.142	-0.800	8.342	-0.174	0.188	0.362	23.045
3	A	N_2O_3	-8.654	-0.800	7.854	-0.140	0.188	0.328	23.946
4	U2	N_2O_3	-9.910	-0.800	9.110	-0.147	0.188	0.335	27.195
5	T	N_2O_3	-9.441	-0.800	8.641	-0.123	0.188	0.311	27.786
6	U1	N_2O_3	-9.710	-0.800	8.910	-0.126	0.188	0.314	28.377
7	N_2O_3	U2	-11.109	-0.415	10.694	-0.051	0.202	0.253	42.268
8	N_2O_3	N_2O_3	-11.109	-0.800	10.309	-0.051	0.188	0.239	43.135
9	N_2O_3	U1	-11.109	-0.511	10.598	-0.051	0.171	0.222	47.738
10	N_2O_3	T	-11.109	-0.475	10.634	-0.051	0.169	0.220	48.336
11	N_2O_3	G	-11.109	-0.206	10.903	-0.051	0.172	0.223	48.892
12	N_2O_3	C	-11.109	-0.344	10.765	-0.051	0.161	0.212	50.778
13	N_2O_3	A	-11.109	-0.213	10.896	-0.051	0.156	0.207	52.637

Table 6. Interactions between SO_2 with nitrogenous bases in cross bands.

Interaction number	Gives lectron cloud	Get lectron cloud	HOMO	LUMO	BG	E-	E+	EP	ETC
1	C	SO_2	-9.142	1.531	10.673	-0.174	0.248	0.422	25.290
2	G	SO_2	-8.537	1.531	10.068	-0.15	0.248	0.398	25.295
3	A	SO_2	-8.654	1.531	10.185	-0.14	0.248	0.388	26.249
4	U2	SO_2	-9.910	1.531	11.441	-0.147	0.248	0.395	28.964
5	SO_2	U2	-10.552	-0.415	10.137	-0.147	0.202	0.349	29.045
6	T	SO_2	-9.441	1.531	10.972	-0.123	0.248	0.371	29.573
7	U1	SO_2	-9.710	1.531	11.241	-0.126	0.248	0.374	30.056
8	SO_2	SO_2	-10.552	1.531	12.083	-0.147	0.248	0.395	30.589
9	SO_2	U1	-10.552	-0.511	10.041	-0.147	0.171	0.318	31.575
10	SO_2	T	-10.552	-0.475	10.077	-0.147	0.169	0.316	31.888
11	SO_2	G	-10.552	-0.206	10.346	-0.147	0.172	0.319	32.432
12	SO_2	C	-10.552	-0.344	10.208	-0.147	0.161	0.308	33.143
13	SO_2	A	-10.552	-0.213	10.339	-0.147	0.156	0.303	34.122

Table 6 shows the interactions between SO_2 with nitrogenous bases in cross bands. The ETC = 26.471, (Table 4 A:T) and ETC = 26.249 (Table 6 A: SO_2) are nearly equal. This comparison indicates that the SO_2 competes with A by T. This competition allows SO_2 can be confused with the A. The probability of that this confusion causes a mutation, is very high.

The ETC = 25.827 (Table 4 C:G) and ETC = 25.290 of (Table 6 C:SO_2) are similar and can also cause confusion.

Table 7 Interactions between CO_2 with nitrogenous bases in cross bands.

Interaction number	Gives electron cloud	Get electron cloud	HOMO	LUMO	BG	E-	E+	EP	ETC
1	C	CO_2	-9.142	1.037	10.179	-0.174	0.164	0.338	30.115
2	G	CO_2	-8.537	1.037	9.574	-0.150	0.164	0.314	30.490
3	A	CO_2	-8.654	1.037	9.691	-0.140	0.164	0.304	31.878
4	U2	CO_2	-9.910	1.037	10.947	-0.147	0.164	0.311	35.199
5	T	CO_2	-9.441	1.037	10.478	-0.123	0.164	0.287	36.508
6	U1	CO_2	-9.710	1.037	10.747	-0.126	0.164	0.290	37.058
7	CO_2	U2	-12.735	-0.415	12.320	-0.072	0.202	0.274	44.965
8	CO_2	U1	-12.735	-0.511	12.224	-0.072	0.171	0.243	50.306
9	CO_2	T	-12.735	-0.475	12.260	-0.072	0.169	0.241	50.873
10	CO_2	G	-12.735	-0.206	12.529	-0.072	0.172	0.244	51.350
11	CO_2	C	-12.735	-0.344	12.391	-0.072	0.161	0.233	53.182
12	CO_2	A	-12.735	-0.213	12.522	-0.072	0.156	0.228	54.923
13	CO_2	CO_2	-12.735	1.037	13.772	-0.072	0.164	0.236	58.357

Table 7 shows the interactions between CO_2 with nitrogenous bases in cross bands. The ETC

= 26.471, (Table 4 A:T) and ETC = 30.115 (Table 7 A: CO_2) are nearly equal. This comparison indicates that the CO_2 competes with A by T. This competition allows CO_2 can be confused with the A. The probability of that this confusion causes a mutation, is very high.

Table 8 shows the interactions between CO with nitrogenous bases in cross bands. The ETC = 26.471, (Table 4 A:T) and ETC = 33.252 (Table 8 C:CO) are the option more probable. This comparison indicates that the CO competes with A by T. This competition allows CO can be confused with the A. The probability of that this confusion causes a mutation, is high.

Table 8 Interactions between CO with nitrogenous bases in cross bands.

Interaction number	Gives electron cloud	Get electron cloud	HOMO	LUMO	BG	E-	E+	EP	ETC
1	C	CO	-9.142	1.000	10.142	-0.174	0.131	0.305	33.252
2	G	CO	-8.537	1.000	9.537	-0.150	0.131	0.281	33.940
3	A	CO	-8.654	1.000	9.654	-0.140	0.131	0.271	35.624
4	U2	CO	-9.910	1.000	10.910	-0.147	0.131	0.278	39.245
5	T	CO	-9.441	1.000	10.441	-0.123	0.131	0.254	41.106
6	U1	CO	-9.710	1.000	10.710	-0.126	0.131	0.257	41.673
7	CO	U2	-13.028	-0.415	12.613	-0.057	0.202	0.259	48.698
8	CO	U1	-13.028	-0.511	12.517	-0.057	0.171	0.228	54.899
9	CO	T	-13.028	-0.475	12.553	-0.057	0.169	0.226	55.544
10	CO	G	-13.028	-0.206	12.822	-0.057	0.172	0.229	55.991
11	CO	C	-13.028	-0.344	12.684	-0.057	0.161	0.218	58.183
12	CO	A	-13.028	-0.213	12.815	-0.057	0.156	0.213	60.164
13	CO	CO	-13.028	1.000	14.028	-0.057	0.131	0.188	74.617

Table 9 shows the interactions between O_3 with nitrogenous bases in cross bands. The ETC = 26.471, (Table 4 A:T) and ETC = 34.240 (Table 9 C: O_3) are the option more probable. This comparison indicates that the O_3 competes with A by T. This competition allows O_3 can be confused with the A. The probability of that this confusion causes a mutation, is high.

Table 9 Interactions between O_3 with nitrogenous bases in cross bands.

Interaction number	Gives electron cloud	Get electron cloud	HOMO	LUMO	BG	E-	E+	EP	ETC
1	C	O_3	-9.142	-0.616	8.526	-0.174	0.075	0.249	34.240
2	G	O_3	-8.537	-0.616	7.921	-0.150	0.075	0.225	35.203
3	A	O_3	-8.654	-0.616	8.038	-0.140	0.075	0.215	37.385
4	U2	O_3	-9.910	-0.616	9.294	-0.147	0.075	0.222	41.864
5	T	O_3	-9.441	-0.616	8.825	-0.123	0.075	0.198	44.569
6	U1	O_3	-9.710	-0.616	9.094	-0.126	0.075	0.201	45.242
7	O_3	U2	-13.008	-0.415	12.593	-0.034	0.202	0.236	53.359

8	O_3	U1	-13.008	-0.511	12.497	-0.034	0.171	0.205	60.960
9	O_3	T	-13.008	-0.475	12.533	-0.034	0.169	0.203	61.737
10	O_3	G	-13.008	-0.206	12.802	-0.034	0.172	0.206	62.144
11	O_3	C	-13.008	-0.344	12.664	-0.034	0.161	0.195	64.942
12	O_3	A	-13.008	-0.213	12.795	-0.034	0.156	0.190	67.341
13	O_3	O_3	-13.008	-0.616	12.391	-0.034	0.075	0.109	113.683

Table 10 shows the interactions between Pb with nitrogenous bases in cross bands. The ETC = 26.471, (Table 4 A:T) and ETC = 72.597 (Table 10 C:Pb) are the option more probable. This comparison indicates that the Pb competes with A by T. This competition allows Pb can be confused with the A. The probability of that this confusion causes a mutation, is high.

Table 10: Interactions between Pb with nitrogenous bases in cross bands.

Interaction number	Gives electron cloud	Get electron cloud	HOMO	LUMO	BG	E-	E+	EP	ETC
1	C	Pb	-9.142	5.087	14.229	-0.174	0.022	0.196	72.597
2	G	Pb	-8.537	5.087	13.624	-0.150	0.022	0.172	79.209
3	A	Pb	-8.654	5.087	13.741	-0.140	0.022	0.162	84.821
4	U2	Pb	-9.910	5.087	14.997	-0.147	0.022	0.169	88.740
5	U1	Pb	-9.710	5.087	14.797	-0.126	0.022	0.148	99.980
6	Pb	U2	-18.626	-0.415	18.211	0.020	0.202	0.182	100.061
7	T	Pb	-9.441	5.087	14.528	-0.123	0.022	0.145	100.193
8	Pb	U1	-18.626	-0.511	18.115	0.020	0.171	0.151	119.968
9	Pb	G	-18.626	-0.206	18.420	0.020	0.172	0.152	121.185
10	Pb	T	-18.626	-0.475	18.151	0.020	0.169	0.149	121.819
11	Pb	C	-18.626	-0.344	18.282	0.020	0.161	0.141	129.660
12	Pb	A	-18.626	-0.213	18.413	0.020	0.156	0.136	135.390
13	Pb	Pb	-18.626	5.087	23.713	0.020	0.022	0.002	11856.550

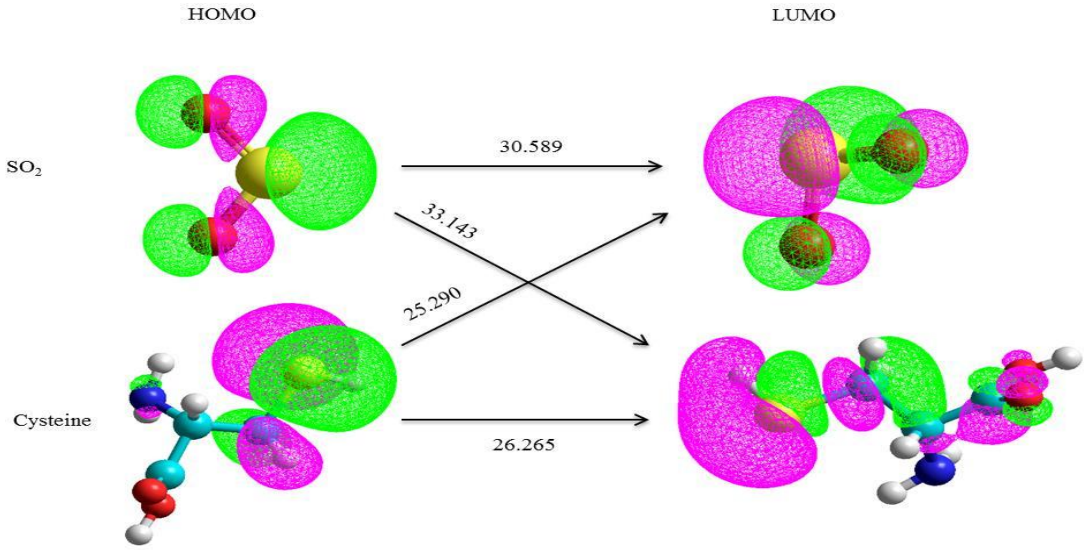

Fig. 2 Interactions between SO_2 with C in cross bands

IV. CONCLUSIONS

We calculated the electronic interactions between molecules of the same chemical species of air pollutants, Nitrogen bases or DNA and RNA. The interplay G:G is the most stable (ETC = 25.872) of all (Table 1) in concordance with the research by Lane [25]. The interaction Pb:Pb is the least stable (ETC = 11856.550). The major unstable interactions are the Pb, CO and O_3, because of this instability can attack anyone of nitrogenous bases, mainly.

We calculated the interactions of cross-bands (Table 2) of the nitrogenous bases. This calculation was according to with the Lane prediction in 1995[20]. We observed the lower ETC = 25.872 belongs to the interaction G:G. This interaction is a mispair occurring DNA or RNA.

As the principal contribution of this study, it can be inferred that C can be confused with the N_2O_3, G can be confused with SO_2; CO_2; CO; O_3 and with the Pb in the genesis of RNA. Because the similar value of ETC of C:G.

With these findings, another avenue to explain the oncogenic and mutagenic effects of N_2O_3, SO_2, CO_2, CO, O_3 and the Pb on the human body are proposed in conjunction with the novel ETC method.

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