

A THEORETICAL STUDY FOR E_2H_2 , E_2H_2AuCl , $E_2H_2(AuCl)_2$ COMPLEXES (E = N–Bi): GEOMETRIES, ATOMS IN MOLECULES, AND NATURAL BOND ORBITAL ANALYSES

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ABSTRACT

The bonding in and stability of dimeric group 15-compounds of the general formula E_2R_2 has been investigated in the past mainly with E = N, P and R = H, CH₃. In this study, we extend these investigations to all group 15-elements E with E = N, P, As, Sb, Bi and analyze the character of the E-E bond for E_2H_2 compounds with the aid of Atoms in Molecule (AIM) and natural bond orbital (NBO). We carried out a comprehensive-theoretical investigation of covalent E_2H_2 compounds and the changes in bonding electron density upon mono- and di-auration. The theoretical results clearly show that the N-N bond in N_2H_2 gets longer upon complexation with AuCl while the P-P-, As-As-, Sb-Sb- and Bi-Bi-bonds exhibit the opposite trend, although the E-E Wiberg bond indices (WBI) decrease upon auration. The condition of a negative total energy ($H(r) < 0$) in the bonding region holds for all E-E bonds of molecules in the AIM analysis. All complexes E_2H_2 , E_2H_2AuCl , $E_2H_2(AuCl)_2$ complexes (E = N–Bi) are suitable targets for synthesis which would open up completely new perspectives for experimental research.

Keywords: atoms in molecules (AIM), natural bond orbital (NBO), bonding electron density, mono-and di-auration.

1. INTRODUCTION

The experimental research for investigating the properties of group-15 double bond contraction upon mono-and di-auration of E_2R_2 with E = N, P and R = H, CH₃ compounds include X-Ray, NMR spectroscopy and neutron diffraction has been studied [1]. After that, the recent chemical bonding for complexes of the group-15 elements have been synthesized by adding phenyl, hydrogen or methyl groups in order to investigate the stability of the unusual bonding modes [2]. These compounds have also been the subject of several theoretical efforts which focused on relative stabilities and rotational barriers, and also on the comparative performance of different computational methods [3].

The AIM methodology has offered a unique tool to get insight into the concept of the chemical bond and the bond strength in terms of electron density distribution [4]. The definition

of the chemical bond is based on the existence of a bond critical point (bcp), extreme of density and the corresponding bond path linking two nuclei of neighboring atoms through a gradient path. At the bond critical point, the gradient of electron density distribution $\Delta\rho(r)$ in the region of two atoms bond always changes between positive and zero. It has been indicated that the $\Delta\rho(r)$ provides a qualitative measure for the accumulation of the electron density in bonding region and the bonding models in which the existence of a covalent bond is dependent upon a finite bonding electron density $\Delta\rho(r)$ gives somewhat dubious [5]. The natural bond orbital (NBO) procedure uses only the information in the atomic orbital overlap and density matrices, and consists of two basis steps: an orthogonalization of the atomic orbital basis to form the natural atomic orbitals (NAOs), and a bond orbital transformation from the NAO set to the final set of NBOs [6].

In order to further explain the chemical bonding in E-E double bond of E_2H_2 compounds ($E = N-Bi$) that carry mono- and di-auration, we used the methods of AIM and NBO analyses which were proposed for study of intermolecular interactions. The points of view that we consider the geometries and energies of E_2H_2 upon mono- and di-auration with the hydrogen in compounds and further explain the nature chemical bond of E-E double bonds in AIM and NBO analyses. The computational assessment of the electronic structure for this study present indicate a rather comprehensive theoretical data base and provide many point of comparison with future experimental studies.

2. COMPUTATIONAL METHODS

We optimized geometries and computed energies for all the molecules at the four different methods BP86 [7], B3LYP [8], M05 [9], and M05-2X [10] with the basis set def2-TZVPP [11] using the Gaussian03 [12] in order to find minima on the energy potential surface (EPS). Vibrational frequencies have also been calculated at the same level of theory to confirm that the structures are minima on the EPS.

The topological analyses of electron densities most of all bonds and wave functions were obtained using the WFN option through single-point calculations. The electron density was analyzed with the AIMPACK set of program using the wave function as input parameters [13] at the BP86 [7] /def2-TZVPP level of theory. The level of theory is denoted as BP86/def2-TZVPP and used for the calculation of the Wiberg bond orders which was analyzed using the natural bond orbital (NBO) program [14] available in Gaussian 03.

3. RESULTS AND DISCUSSION

The optimized geometries structures of E_2H_2 (*cis-trans*) compounds at the four different methods BP86, B3LYP, M05, and M05-2X with basis set def2-TZVPP are shown in Figure 1 and Table 1. Experimental geometry of N_2H_2 is only given [14]. The calculated results in Table 1 show that bond lengths of N-N, N-H and the bond angle of H-N-N are nearly similar among difference methods, the experimental value of N_2H_2 for N-N (1.252 Å) and N-H (1.028 Å) bond length are slightly longer than the theoretical data. The P-P bond length is significantly longer than N-N bond length and the E-E bonds increase for the heavier homologues.

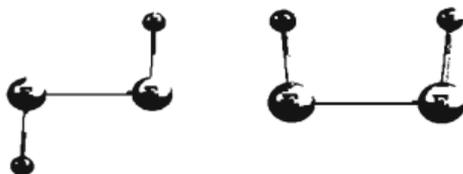


Figure 1. Optimized structures of E_2H_2 (cis-trans) at the BP86, B3LYP, M05, M05-2X levels with the basic set def2-TZVPP.

Table 1 shows that the bond length of As-As is longer than P-P bond length and becomes longer from As-As to Bi-Bi bond. Besides, the other bond lengths and bond angles are also not big difference among these compounds. Note that the values of related energies are observed similar trends we also found that almost of *trans* structures are lower in energies than *cis* structures. From those, we choose the *trans* structures of E_2H_2 compounds upon mono- and di-auration and the level of theory BP86/ *def2-TZVPP* for continuously investigating in the following studies.

The referee asked the reason for applying different methods and for selecting the BP86/ *def2-TZVPP* level among 4 different levels of theory while they exhibit nearly the same values of bond lengths and energies, we would like to explain as follows: As mentioned in the abstract, in this study, we extend these investigations to all group 15-elements E with $E = N, P, As, Sb, Bi$ and analyze the character of the E-E bond for E_2H_2 compounds with the aid of Atoms in Molecule (AIM) and natural bond orbital (NBO). This is because the finding suggest that it would be worth investigating the E_2H_2 compounds ($E = N-Bi$) that carry mono- and di-auration, which may exist, but have not yet been synthesized, except for the experimental study for N_2H_2 compound. Furthermore, to the best of our knowledge, the present work is the first detailed study of the geometries and bonding situation of the E_2H_2 , E_2H_2AuCl , $E_2H_2(AuCl)_2$ complexes ($E = N-Bi$). Originally we only used the B3LYP level with the basis set def2-TZVPP and then we decided to extend these calculations to BP86, M05, and M05-2X levels with the same basis set in order to find out the significantly differences among those methods. In the end, we realized that although there are not different much for structures and energies among the four methods but the BP86/ *def2-TZVPP* level would be chosen for further investigating due to the higher accuracy with the $c2h$ point group symmetry of E_2H_2 molecules.

Table 1. Optimized geometries of E_2H_2 compounds with $E = N-Bi$ at BP86, B3LYP, M05, M05-2X levels with basis set def2-TZVPP, and the calculated relative energies [kcal/mol] with different methods.

Molecule	Method	$d(E-E)^{[a]}$	$d(E-H)^{[a]}$	$\alpha(H-E-E)^{[b]}$	$E_{rel}^{[c]}$
N_2H_2 -cis	BP86	1.245	1.052	112.8	5.0
	B3LYP	1.234	1.039	112.9	5.4
	M05	1.231	1.035	112.7	5.6
	M05-2X	1.226	1.031	112.4	6.0
	BP86	1.249	1.045	106.3	0

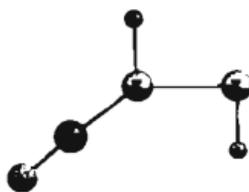
N_2H_2 - <i>trans</i>	B3LYP	1.235	1.033	107.0	0
	M05	1.234	1.030	106.5	0
	M05-2X	1.226	1.027	107.1	0
	<i>Exp[15]</i>	1.252 ± 0.002	1.028 ± 0.005	106.9 ± 0.5	
P_2H_2 - <i>cis</i>	BP86	2.052	1.435	99.3	3.5
	B3LYP	2.037	1.422	99.7	3.5
	M05	2.033	1.424	98.9	3.8
	M05-2X	2.021	1.417	98.9	3.6
P_2H_2 - <i>trans</i>	BP86	2.043	1.438	93.6	0
	B3LYP	2.029	1.426	94.2	0
	M05	2.022	1.427	93.2	0
	M05-2X	2.012	1.420	94.0	0
As_2H_2 - <i>cis</i>	BP86	2.280	1.540	96.9	2.7
	B3LYP	2.266	1.529	97.5	2.7
	M05	2.245	1.530	97.6	2.8
	M05-2X	2.238	1.520	97.3	2.7
As_2H_2 - <i>trans</i>	BP86	2.269	1.546	91.9	0
	B3LYP	2.256	1.533	92.6	0
	M05	2.235	1.534	92.6	0
	M05-2X	2.230	1.525	92.8	0
Sb_2H_2 - <i>cis</i>	BP86	2.669	1.728	94.5	2.1
	B3LYP	2.657	1.717	95.1	2.1
	M05	2.670	1.729	95.0	2.3
	M05-2X	2.598	1.703	96.0	2.0
Sb_2H_2 - <i>trans</i>	BP86	2.655	1.734	90.4	0
	B3LYP	2.644	1.722	91.1	0

	M05	2.656	1.735	90.8	0
	M05-2X	2.590	1.708	91.9	0
	BP86	2.823	1.808	94.0	1.9
Bi_2H_2 -cis	B3LYP	2.813	1.798	94.6	1.9
	M05	2.873	1.826	93.9	2.3
	M05-2X	2.729	1.772	94.4	2.0
	BP86	2.809	1.815	89.7	0
Bi_2H_2 -trans	B3LYP	2.800	1.805	90.3	0
	M05	2.855	1.834	89.7	0
	M05-2X	2.720	1.781	90.5	0

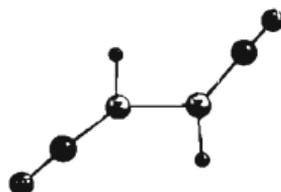
[a]: in Å; [b]: in degree; [c]: in kcal/mol



E_2H_2
 $d(N-N) = 1.249$
 $d(P-P) = 2.043$
 $d(As-As) = 2.269$
 $d(Sb-Sb) = 2.655$
 $d(Bi-Bi) = 2.809$



E_2H_2AuCl
 $d(N-N) = 1.258$
 $d(P-P) = 2.033$
 $d(As-As) = 2.256$
 $d(Sb-Sb) = 2.636$
 $d(Bi-Bi) = 2.791$



$E_2H_2(AuCl)_2$
 $d(N-N) = 1.282$
 $d(P-P) = 2.031$
 $d(As-As) = 2.249$
 $d(Sb-Sb) = 2.625$
 $d(Bi-Bi) = 2.781$

Figure 2. Optimized geometries of E_2H_2 (trans), E_2H_2AuCl , $E_2H_2(AuCl)_2$ compounds ($E = N-Bi$) with point group symmetries: c_{2h} for E_2H_2 (trans-planar) and c_s for E_2H_2 with mono- and di-auration at BP86/def2-TZVPP level. Bond lengths are given in Å.

Exp [15] of N-N bond = 1.252 ± 0.002 .

The optimized geometries of E_2H_2 , E_2H_2AuCl , $E_2H_2(AuCl)_2$ complexes with $E = N-Bi$ together with the calculated values for the bond lengths are shown in the Figure 2. The equilibrium structures of the systems possess the main E-E bonds. All complexes are experimentally unknown except for geometry of N_2H_2 [15]. Figure 2 shows that the E-E bond increases from the lighter to the heavier complexes. Note that the N-N bond length in N_2H_2 is the shortest bond (1.249 Å) and the bond lengths in mono- and di-auration increase from 1.258 Å in E_2H_2AuCl to 1.282 Å in $E_2H_2(AuCl)_2$, whereas the bond lengths of P-P slightly decrease from

P_2H_2 (2.043 Å) to $P_2H_2(AuCl)_2$ (2.031 Å) and this trend is also observed for compounds of As, Sb, and Bi.

We continue investigating the nature chemical bond of E-E double bonds using the AIM method approach for the neutral complexes $E_2H_2(trans)$, E_2H_2AuCl and $E_2H_2(AuCl)_2$. It is pointed out that the AIM approach relies on an analysis of the topological properties of the charge density $\Delta\rho(r)$ and its quality depends on the computational level chosen. In this case, we analyzed the $\rho(r)$ directly from the sign of the Laplacian of density which is determined by relationship with $\nabla^2\rho(r) = \lambda_1 + \lambda_2 + \lambda_3$ ($\lambda_1 < 0$, $\lambda_2 < 0$ and $\lambda_3 > 0$ are the three nonzero eigenvalues of the Hessian matrix of $\rho(r)$). If the electrons are locally concentrated at a particular point and shared by both nuclei in covalent interaction, then $\nabla^2\rho(r)$ is negative. In contrast to this, the values of $\nabla^2\rho(r)$, if the electron are depleted from the bond critical point (bcp) and concentrated in each of the atomic basin (closed-shell interaction), $\nabla^2\rho(r)$ is positive. Both the gradient and the Laplacian of the charge density, $\nabla\rho$, and $\nabla^2\rho$, respectively, can be analyzed and provide complementary information on bonds.

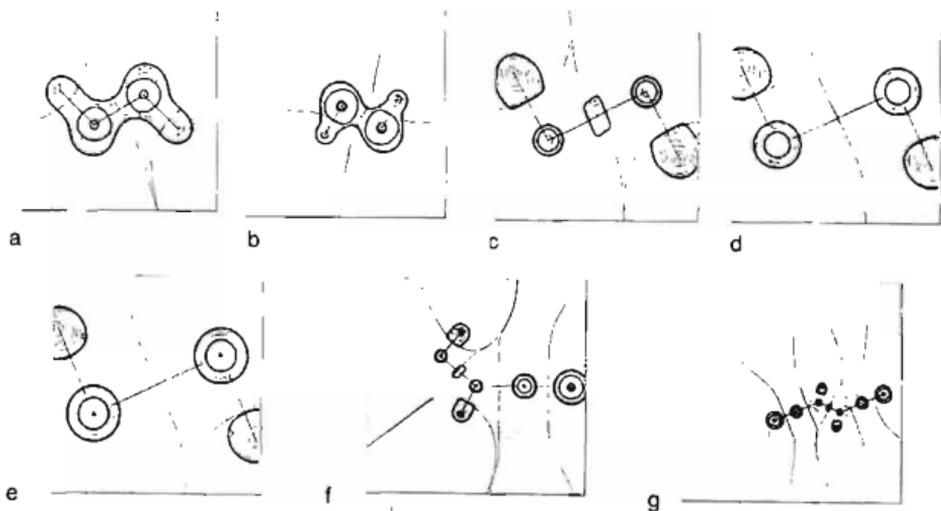


Figure 3. Contour line of diagram of Laplace field and the path of the charge density $\nabla^2\rho$ in E_2H_2 (trans) (a: N_2H_2 ; b: P_2H_2 ; c: As_2H_2 ; d: Sb_2H_2 ; e: Bi_2H_2); f: As_2H_2AuCl and g: $As_2H_2(AuCl)_2$.

The critical points, $\nabla\rho$, give information about the existence of bonds, while the sign of $\nabla^2\rho$ at the same point reflects the kind of the interaction, namely the Laplacian of the charge density, $\nabla^2\rho$, is negative at the critical point for covalent interactions, and it is positive for closed shell interaction, such as E-H, E-Au or Au-Cl bonds. The plot of the gradient of the charge density, $\nabla\rho$, in the plane of the E_2H_2 , E_2H_2AuCl , and $E_2H_2(AuCl)_2$ molecules interaction are given in the Figure 3. The map of the Laplacian and the path of the charge density $\nabla^2\rho$ in the $H\dots E\dots E\dots H$; $H\dots E\dots E\dots H$ with $E\dots Au\dots Cl$, and $H\dots E\dots E\dots H$ with $(E\dots Au\dots Cl)_2$ planes is also shown.

There are critical bonds between each set of two atoms defining a covalent bond and Wiberg bond orders of the E-E bonds which are shown in Table 2. The features of the most

relevant critical points for those bonds are suitable for the bonds of investigated complexes. Table 2 shows that the laplacian at N-N, P-P, and As-As bond critical points are negative and become smaller and bigger in all of them. They are negative at the Sb-Sb bond critical points of Sb₂H₂ and become positive in Sb₂H₂AuCl (0.122 e.Å⁻⁵) to -0.075 e.Å⁻⁵ in Sb₂H₂(AuCl)₂. In contrast to this, the laplacian values are always positive at Bi-Bi bond critical points from Bi₂H₂ (0.946 e.Å⁻⁵) to Bi₂H₂(AuCl)₂ (1.030 e.Å⁻⁵). The Wiberg bond orders of N-N -, P-P-, As-As-, Sb-Sb- and Bi-Bi- bonds are not different and especially they decrease upon mono- and di-auration in the compounds.

We realize that one possibility to analyze these changes in the bonding region is provide by the relation $2G(r) + V(r) = \frac{1}{2} \nabla^2 \rho(r)$, derived by the Bader theory [15] which connects the kinetic energy density $G(r)$ and the potential energy density $V(r)$ with the Laplace field of $\rho(r)$. Point wise analysis of $G(r)$ and $V(r)$ indicates that for covalent bonds the local energy density $H(r) = G(r) + V(r)$ at sites of maximum concentration of $\rho(r)$ is always negative. This also applies to the E-E bonds in our current study. Figure 3 clearly show that the Laplacian at N-N, P-P, and As-As bonds critical points in *a*, *b*, and *c* are negative but they are nearly zero for Sb-Sb and Bi-Bi bonds in *d* and *e*. The Laplacian at As-As bond critical points is small negative in both cases of As₂H₂AuCl and As₂H₂(AuCl)₂ in *f* and *g*. The AIM pictures of the other compounds upon mono- and di-auration are quite similar compared with As compound and they are not shown in figure 3.

Table 2. Characterization of covalent bonds by total electron density and Wiberg bond indices (WBI) of E₂H₂(trans), E₂H₂AuCl, and E₂H₂(AuCl)₂ molecules with E = N – Bi. [a]: e.Å⁻³; [b]: e.Å⁻⁵; [c]: Hartree.Å⁻³.

Molecule	Bond	$\rho(r)$ [a]	$\nabla^2 \rho(r)$ [b]	$H(r)$ [c]	WBI
N ₂ H ₂	N-N	3.227	-32.280	-4.286	2.065
N ₂ H ₂ AuCl	N-N	2.896	-23.630	-3.305	1.840
N ₂ H ₂ (AuCl) ₂	N-N	3.067	-25.593	-3.662	1.593
P ₂ H ₂	P-P	0.988	-5.623	-0.678	2.046
P ₂ H ₂ AuCl	P-P	0.977	-1.851	-0.878	1.808
P ₂ H ₂ (AuCl) ₂	P-P	1.015	-7.178	-0.763	1.642
As ₂ H ₂	As-As	0.736	-1.573	-0.388	2.029
As ₂ H ₂ AuCl	As-As	0.728	-1.195	-0.379	1.798
As ₂ H ₂ (AuCl) ₂	As-As	0.742	-1.501	-0.388	1.624
Sb ₂ H ₂	Sb-Sb	0.494	-0.043	-0.181	2.021

Sb ₂ H ₂ AuCl	Sb-Sb	0.489	0.122	-0.189	1.790
Sb ₂ H ₂ (AuCl) ₂	Sb-Sb	0.502	-0.075	-0.199	1.645
Bi ₂ H ₂	Sb-Sb	0.424	0.946	-0.121	2.017
Bi ₂ H ₂ AuCl	Sb-Sb	0.410	1.121	-0.121	1.753
Bi ₂ H ₂ (AuCl) ₂	Sb-Sb	0.420	1.030	-0.127	1.636

From above results, we can assert that the bond formation is associated with a gain in molecular energy and this gain is a result of the complex interplay of changes in potential and kinetic energy. These also apply to all bonds except for the different Laplacian value of Sb₂H₂AuCl complex. It can be seen in table 2 that the electron density flows out of the inter-nuclear region upon bond formation. Note that the similar trends for the local energy density $H(r)$ are observed for the compounds of P, As, Sb and Bi. Table 2 also shows that the condition $H(r)$ is negative in the bonding region which holds for all covalent bonds in this study. From this it can follow that the N-N bond in N₂H₂ is stronger and shorter than the other bonds while P-P bond in P₂H₂(AuCl)₂ is nearly stronger than P-P bond in P₂H₂ and the As-As, Sb-Sb, and Bi-Bi bonds both change with the same trends in complexes.

4. CONCLUSION

The theoretical results presented in this study clearly show that the N-N bond in N₂H₂ gets longer upon complexation with AuCl while the P-P-, As-As-, Sb-Sb- and Bi-Bi-bonds exhibit the opposite trend, although the E-E Wiberg bond indices (WBI) decrease upon auration. The condition of a negative total energy ($H(r) < 0$) in the bonding region holds for all E-E bonds of molecules in the ADM analysis.

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TÓM TẮT

TÍNH TOÁN LÝ THUYẾT CÁC HỢP CHẤT E_2H_2 , E_2H_2AuCl , $E_2H_2(AuCl)_2$ ($E = N-Bi$): CẤU TRÚC, NGUYÊN TỬ TRONG PHÂN TỬ, VÀ PHÂN TÍCH BẢN CHẤT ORBITAL LIÊN KẾT TỰ NHIÊN

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Bản chất liên kết và tính ổn định của các hợp chất nhóm 15 có công thức chung E_2R_2 với $E = N, P$ và $R = H, CH_3$ đã được nghiên cứu trước đây. Trong nghiên cứu này, chúng tôi mở rộng các tính toán cho tất cả các hợp chất với $E = N, P, As, Sb, Bi$ và phân tích các đặc tính của liên kết chính E-E cho các hợp chất E_2H_2 với bằng các phương pháp nguyên tử trong phân tử (AIM) và phân tích orbital liên kết tự nhiên (NBO). Một nghiên cứu toàn diện bằng tính toán lý thuyết cho các hợp chất cộng hóa trị E_2H_2 và những thay đổi trong mật độ điện tử liên kết trong hợp chất E_2H_2 chứa lẫn lượt $AuCl$ và $(AuCl)_2$ (mono- và di-auration). Kết quả lý thuyết cho thấy độ dài liên kết N-N trong N_2H_2 dài hơn khi tạo phức với $AuCl$ trong khi các liên kết P-P-, As-As-, Sb-Sb và Bi-Bi-, mặc dù các liên kết tính điện Wiberg E-E (WBI) giảm khi hợp chất nghiên cứu tạo phức với $AuCl$ và $(AuCl)_2$. Các điều kiện của tổng năng lượng ($H(r) < 0$) trong vùng liên kết hoàn toàn phù hợp cho tất cả các liên kết E-E của các phân tử trong phân tích AIM. Tất cả các hợp chất E_2H_2 , E_2H_2AuCl , $E_2H_2(AuCl)_2$ với $E = N-Bi$ trong nghiên cứu lý thuyết này hoàn toàn phù hợp để định hướng cho các nghiên cứu thực nghiệm, đặt biệt với hy vọng mở ra nhiều viễn cảnh hoàn toàn mới cho các nghiên cứu về môi trường.

Từ khóa: nguyên tử trong phân tử (AIM), orbital liên kết tự nhiên (NBO), tính toán dựa trên lý thuyết phiếm hàm mật độ; mono- và di-auration.