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# Investigating pseudo Jahn–Teller effect on inter-molecular hydrogen bond in enolic forms of benzonium compounds and analog containing P and As atoms

Elahe Jalali

*Department of Chemistry, Damghan Branch, Islamic Azad University, Damghan, Iran*

## ABSTRACT

This study investigates the effect of Pseudo Jahn-Teller Effect (PJTE) on distortion of hydrogen bonds of high symmetry forms of 1, 3-di (pyridine-2-yl) Benzonium (1) and analog containing P (2) and As (3) atoms. The results of B3LYP/6-311++G** method indicate that the forms having inter-molecular hydrogen bond in compounds (1)-(3) with C2V symmetry have the highest value of ground state electron configuration energy (ECE). Applying normal coordination, C2V high symmetry forms turn into Cs low symmetry forms. C2V high symmetry form have two virtual frequencies with b2 and b1 symmetry. In Pseudo Jahn-Teller problem, compounds (1)-(3) are in in the forms of (A1+B2) ⊗ b2 and (A1+B1) ⊗ b1, and the energy difference between reference combining levels (Δ) reduces from compound (1)-(3).

**KEY WORDS:** PSEUDO JAHN-TELLER EFFECT, HYDROGEN BOND, INTER-MOLECULAR DISTORTION, COMPUTATIONAL CHEMISTRY, GAUSSIAN SOFTWARE

## INTRODUCTION

In recent years, increasing growth of quantum chemistry and emergence of high-speed computers has led to creation of a new field in chemistry, called computational chemistry, in which computers are used as an empirical device. The main objective of this newly found field in the chemistry science is just proving the results related to chemistry problems, and the computational methods used today are one of the most powerful tools to study the mechanism of reactions and predict the characteristics of stable molecules, namely their nature, formation, bond energy, etc. (Hamilton *et al.* 1962).

In certain chemical compounds, hydrogen bond has been the subject of many researches because of its significant importance. The significant role of hydrogen
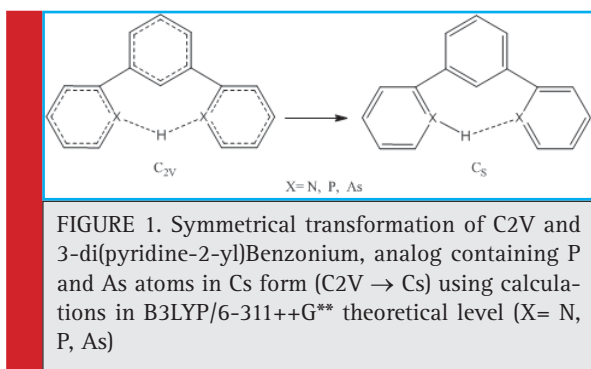
bond in chemical and bio-chemical phenomena, as well as the nature of this bond's structure, has scientifically made it remarkable and worthy of further scrutiny and research. Phenomena affected by hydrogen bond are extensively found in daily life. These phenomena can go under specialist assessment by empirical techniques (Pimcntel and Clellan, 1976).

Inter-molecular hydrogen bond (IMHB) exists in many organic molecules and bio-molecules such as carbohydrates, hormones, and proteins. Furthermore, this type of bond determines the configuration of many molecules, and it is because of such bond that proteins have unique configurations. An important parameter in classifying systems with hydrogen bond is its strength. Structurally, this strength is determined by parameters such as the distance between two electronegative atoms (A...B), length of hydrogen bond (H...B), length of covalent bond (A–H), and bond angle (AˆHˆB), as well as thermodynamic parameters such as enthalpy of formation ($\Delta Hf$), entropy of formation ($\Delta Sf$), and Gibbs free energy ($\Delta Gf$) (Pauling, 1960; Speakman, 1975). These empirical methods experienced cannot measure hydrogen bond strength, or at least have limited applications. Theoretical and computational methods are more efficient and comprehensive in this context, in which molecules can be optimized in any structural and electron mode in terms of energy. These methods, which seem necessary for measuring inter-molecular hydrogen bond energy, have also significantly developed after emergence of ultra-modern computers with high speed and performance.

Reviewing the literature revealed that no reports have yet been published related to the objectives of this study. Given the fact that hydrogen bond is one of the effective factors in human life, its effect has been examined in 1,3-di(pyridine-2-yl)Benzonium (1) and analog containing P (2) and As (3) atoms by pseudo Jahn-Teller analysis using high level B3LYP/6-311++G** theoretical method.

It is expected that the pseudo Jahn-Teller effect can describe the transformation of C2V high symmetry structures to Cs low symmetry structures in the following compounds (Figure 1):



FIGURE 1. Symmetrical transformation of C2V and 3-di(pyridine-2-yl)Benzonium, analog containing P and As atoms in Cs form (C2V → Cs) using calculations in B3LYP/6-311++G** theoretical level (X= N, P, As)

(1) 1,3-di(pyridine-2-yl)Benzonium (2) and analog containing P atoms (3) and As atoms

It was found that compounds (1)-(3) mentioned above have C2V high symmetry configuration. By Q transformations, the first three compounds with C2V high symmetry configuration turn into Cs configuration.

This study carefully investigates the important issue of ground state electron mixing in electron exited state in the direction of applying normal coordination describing leaving high symmetry and transforming into low symmetry. The major cause of deformation was the pseudo Juan-Teller effect, which was created by combining the ground state and excited states.

Since the electron ground state of these compounds is not aligned, it is obvious that all deformations observed from linear configuration with the highest symmetry is due to pseudo Juan-Teller effect (Bersuker, 2006). Generally, the pseudo Juan-Teller effect is associated with non-aligned stated of any system, Juan-Teller effect is associated with aligned stated of non-linear molecules, and Renner-Teller effect is associated with aligned stated of linear molecules (Bersuker, 2001).

All of these effects are general and unique forms, each describing symmetrical instability and many other issues briefly discussed in the following.

## MATERIAL AND METHODS

### COMPUTATIONAL METHODOLOGY

First, the molecular form, written based on Zmatrix, will be drawn and numbered, given the desired symmetry. Then, the optimal molecular structure and its negative frequency will be calculated using Gaussian 03 & 98 software. Then, DFT hybrid-based method (B3LYP) with 6-311++G** base series will be used for all desired compounds.

Computational time depends on the Density Function Theory (DFT). TD-DFT is, for sure, one of the most common tools for investigating the excited levels of molecular systems, which has been used to study the electron configuration of Enolic structures of 1,3-di(pyridine-2-yl)Benzonium and analog containing P and As atoms.

Results of B3LYP/6-311++G** and TD-DFT shows that the major reason for deformation of high symmetry configurations (C2V) to low symmetry configurations (Cs) for these compounds is pseudo Juan-Teller effect, which is created by combining ground state and excited stated. The energy difference ($\Delta$) and pseudo Juan-Teller stability energy between reference stated and $\Delta Ee1$ in these forms (C2V → Cs) is also investigated.

## RESULTS AND DISCUSSION

Quantum mechanics calculations in the B3LYP/6-311++G** initial level was used to examine the structural properties of molecules in compounds (1)-(3).

### 3-1. Investigating pseudo Juan–Teller effect on distortion of 1,3-di(pyridine–2-yl)Benzonium molecule (compound No. 1)

Initial quantum mechanics calculations in the B3LYP/6-311++G** theoretical level showed that 1,3-di(pyridine-2-yl)Benzonium structure has C2V high symmetry, while has low symmetry in Cs point group, whose deviation with high symmetry arrangement is due to pseudo Juan-Teller effects, which is the only source of instability for



FIGURE 2. Symmetrical transformation of C2V in 1,3-di(pyridine-2-yl)Benzonium (C2V → Cs) using calculations in B3LYP/6-311++G** theoretical level

arrangements with high symmetry in aligned and non-aligned states. Deviations is created by combining the base level A1 and the excited level B2 through displacement of b2, and in another case by combining base level A1 and the excited level B2 through displacement of b1. Pseudo Juan-Teller results in (A1+B2) ⊗ b2 and (A1+B1) ⊗ b1 problems.

The energy difference between ground state and excited level B2 (Figure 3) and between ground state and excited level B1 (Figure4), along with combination of orbitals is 5.35 eV and 5.55 eV, respectively.

1. [Homo – 3 (A2) → Lumo 1(B1), Homu – 2(B1) → Lumo (A2), Homo –1 (A2) → Lumo + 3 (B1)], [Homo – 1 (A1) → Lumo + 5(B1)]
2. [Homo – 7 (A1) → Lumo + 1(B1), Homo – 5(B2) → Lumo (A2)]

Given the reduction of energy difference in your desired compound in B2 symmetry compared to B1, its pseudo Juan-Teller energy would be higher. ΔEe1 also confirms it in this case.

The electron energy of some excited levels for 1,3-di(pyridine-2-yl)Benzonium structure, calculated in B3LYP/6-311++G** theoretical level (eV), is given in Table 1, which indicates that B1 excited level with



FIGURE 3. Initial energy levels calculated (ground state and excited state with B2 symmetry) in 1,3-di(pyridine-2-yl)Benzonium molecule, and their changes by pseudo Juan-Teller effect (first case)



FIGURE 4. Initial energy levels calculated (ground state and excited state with B1 symmetry) in 1,3-di(pyridine-2-yl)Benzonium molecule, and their changes by pseudo Juan-Teller effect (second case)
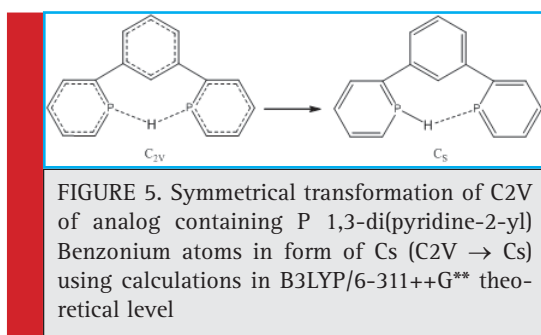
Table 1. Investigating the energy of excited levels (eV) of 1,3-di(pyridine-2-yl)Benzonium in symmetrical transformation (C2V → Cs) (two cases).

| | $B_2$ | $A_1$ | $B_2$ | $A_1$ | $B_2$ | $B_2$ | $A_1$ | $B_1$ |
|---|---|---|---|---|---|---|---|---|
| 1. $C_{16}H_{13}N_2(+1)$ | 3.84 | 3.96 | 3.98 | 4.29 | 5.22 | 5.35 | 5.42 | – |
| 2. $C_{16}H_{13}N_2(+1)$ | 3.87 | 3.10 | 4.01 | 4.32 | 5.25 | – | 5.45 | 5.55 |

Table 2. The thermodynamic functions calculated (enthalpy, Gibbs free energy (Hartree), and entropy (calmil-1k-1)), ground state energy, and their changes in 25°C and 1 atm for compounds ,3-di(pyridine-2-yl)Benzonium, analog containing P and As atoms, using calculations in B3LYP/6-311++G** theoretical level.

| Geometries | H (Hartree) | S (cal mol$^1$K$^{-1}$) | G (Hartree) | $\Delta Ha$ (Hartree) | $\Delta S^a$ (calmol$^1$K$^{-1}$) | $\Delta G^a$ (Hartree) | Eel | $\Delta Eel$ |
|---|---|---|---|---|---|---|---|---|
| 1-C16H13N2(1+). TD 0.0 | –726.618341 | 109.243 | –726.670246 | 0.120568 | 0.0000 | 0.123099 | –726.8782112 | 0.1259201 |
| | | | | (75.66) | | (77.25) | | (79.02) |
| 1- C16H13N2(1+). TD 0.5 | –726.738909 | 114.569 | –726.793345 | 0.0000 | 5.326 | 0.0000 | –727.0041313 | 0.0000 |
| | | | | (0.00) | | (0.00) | | (0.00) |
| 2- C16H13N2(1+). TD 0.0 | –726.618341 | 109.243 | –726.670246 | 0.076013 | 0.000 | 0.076965 | –726.8782112 | 0.0765166 |
| | | | | (47.70) | | (48.30) | | (48.01) |
| 2- C16H13N2(1+). TD 0.4 | –726.694354 | 111.246 | –726.747211 | 0.0000 | 2.003 | 0.000 | –726.9547278 | 0.0000 |
| | | | | (0.00) | | (0.00) | | (0.00) |
| 3- C16H13P2(1+). TD 0.0 | –1299.850127 | 118.706 | –1299.906528 | 0.045676 | 4.414 | 0.043578 | –1300.0992816 | 0.0477544 |
| | | | | (28.66) | | (27.35) | | (29.97) |
| 3- C16H13P2(1+). TD 0.4 | –1299.895803 | 114.292 | –1299.950106 | 0.0000 | 0.0000 | 0.0000 | –1300.147036 | 0.0000 |
| | | | | (0.00) | | (0.00) | | (0.00) |
| 4- C16H13P2(1+). TD 0.0 | –1299.850127 | 118.706 | –1299.906528 | 0.02395 | 0.0000 | 0.024946 | –1300.0992816 | 0.0244918 |
| | | | | (15.03) | | (15.65) | | (15.37) |
| 4- C16H13P2(1+). TD 0.4 | –1299.874077 | 120.804 | –1299.931474 | 0.0000 | 2.098 | 0.000 | –1300.1237734 | 0.0000 |
| | | | | (0.00) | | (0.00) | | (0.00) |
| 5- C16H13As2(1+). TD 0.0 | –5088.839500 | 120.345 | –5088.896680 | 0.03185 | 1.068 | 0.031342 | –5089.0854207 | 0.0346449 |
| | | | | (19.99) | | (19.67) | | (21.74) |
| 5- C16H13As2(1+). TD 0.4 | –5088.871350 | 119.277 | –5088.928022 | 0.0000 | 0.0000 | 0.000 | –5089.1200656 | 0.0000 |
| | | | | (0.00) | | (0.00) | | (0.00) |
| 6- C16H13As2(1+). TD 0.0 | –5088.839500 | 120.345 | –5088.896680 | 0.017477 | 0.0000 | 0.021056 | –5089.0854207 | 0.0189186 |
| | | | | (10.97) | | (13.21) | | (11.87) |
| 6- C16H13As2(1+). TD 0.5 | –5088.856977 | 127.877 | –5088.917736 | 0.0000 | 7.532 | 0.0000 | –5089.1043393 | 0.0000 |
| | | | | (0.00) | | (0.00) | | (0.00) |
| 7- C16H13As2(1+). TD 0.0 | –5088.839500 | 120.345 | –5088.896680 | 0.000686 | 0.0000 | 0.002027 | –5089.0854207 | 0.001695 |
| | | | | (0.43) | | (1.27) | | (1.06) |
| 7- C16H13As2(1+). TD 0.4 | –5088.840186 | 123.167 | –5088.898707 | 0.0000 | 2.822 | 0.0000 | –5089.0871157 | 0.0000 |

FIGURE 5. Symmetrical transformation of C2V of analog containing P 1,3-di(pyridine-2-yl) Benzonium atoms in form of Cs (C2V → Cs) using calculations in B3LYP/6-311++G** theoretical level

an energy about 5.55 eV poorly contributes in creating pseudo Juan-Teller effect.

The value of thermodynamic parameters $\Delta G$, $\Delta H$, $\Delta S$, and $\Delta Ee1$ of the desired compound, shown in Table 2, was calculated using B3LYP/6-311++G** method. The results show that the value of $\Delta Ee1$ for 1,3-di(pyridine-2-yl)Benzonium is 79.02 kCal/mol and 48.01 kCal/mol for B2 symmetry and B1 symmetry, respectively, which implies that the desired compound with B1 symmetry has lower pseudo Juan-Teller stability energy. Since the energy difference between the ground and excited states of B2 is lower than that of B1, its $\Delta Ee1$ is higher, so 1,3-di(pyridine-2-yl)Benzonium with B2 symmetry has higher pseudo Juan-Teller stability energy.

### 3–2. Investigating pseudo Juan–Teller effect on distortion of analog containing P 1,3–di(pyridine–2–yl) Benzonium atom (compound No. 2)

Structural properties of compound No. 2 was examined using B3LYP/6-311++G** theoretical level. The results showed that compound No. 2 has C2V high symmetry, and has low symmetry in point group. Deviations of this arrangement with high symmetry are caused by psuedo Juan-Teller effect, which is the only source of instability for arrangements with high symmetry in aligned and non-aligned states. The deviations are formed as a result of combining the compound of ground state A1 and excited level B2 by displacement b2, and another case as a result of combining the ground state A1 and excited level B1 through displacement b1, i.e., Energy difference between ground state and excited state B2 (first case) and between ground state and excited state B1 (second case) is 5.10 and 4.46 eV, respectively.

1. [Homo – 6 (A2) → Lumo (B1), Homo – 5(B1) → Lumo+1(A2), Homo – 5 (B1) → Lumo + 2 (A2), Homo – 3 (B1) → Lumo + 1(A2), Homo – 2 (A2) → Lumo (B1), Homo – 1(B1) → Lumo + 2 (A2), Homo (A2) – Lumo + 4(B1), Homo (A2) → Lumo + 5 (B1)]
2. [Homo – 4 (B2) → Lumo + 1(A2), Homo – 1(B1) → Lumo + 3 (A1)]

So, pseudo Juan-Teller results in (A1+B2) ⊗ b2 and (A1+B1) ⊗ b1 problems.

Given the reduction in the energy difference of the desired compound in B1 symmetry, it is expected that its pseudo Juan-Teller energy would be higher (regardless of other factors).

Figures 6 and 7 show the energy of ground level and excited levels, as well as the deviations of arrangements with high symmetry due to pseudo Juan-Teller effect.

The electron energy of a number of excited levels for the structure of the compound No. 2, calculated in B3LYP/6-311++G** theoretical level (eV), is reported in Table 3, which shows that B2 excited level with an approximate energy of 5.10 eV (first case) and B1 excited level with an approximate energy of 4.46 eV (first case) contribute in making pseudo Juan-Teller effect.

The value of thermodynamic parameters $\Delta G$, $\Delta H$, $\Delta S$, and $\Delta Ee1$ of the desired compound, shown in Table 2, was calculated using B3LYP/6-311++G** method. The results show that the value of $\Delta Ee1$ for compound No. 2 is 29.97 kCal/mol and 15.37 kCal/mol for B2 symmetry and B1 symmetry, respectively, which implies that the desired compound with B1 symmetry has lower pseudo Juan-Teller stability energy, however, the energy difference between reference states has decreased.



FIGURE 6. Initial energy levels calculated (ground state and excited state with B2 symmetry) in analog containing P 1,3-di(pyridine-2-yl)Benzoniumatoms, and their changes by pseudo Juan-Teller effect (first case)

FIGURE 7. Initial energy levels calculated (ground state and excited state with B1 symmetry) in analog containing P 1,3-di(pyridine-2-yl)Benzoniumatoms, and their changes by pseudo Juan-Teller effect (second case)

Table 3. Investigating the energy of excited levels (eV) of analog containing P 1,3-di(pyridine-2-yl)Benzonium atoms in symmetrical transformation (C2V → Cs) (two cases).

| | $B_2$ | $A_1$ | $B_2$ | $A_2$ | $B_1$ | $B_2$ | $A_1$ | $B_2$ |
|---|---|---|---|---|---|---|---|---|
| 1. $C_{16}H_{13}P_2(+1)$ | 3.15 | 3.32 | 3.71 | 4.33 | – | 4.55 | 4.94 | 5.10 |
| 2. $C_{16}H_{13}P_2(+1)$ | 3.18 | 3.36 | 3.74 | 4.38 | 4.46 | 4.58 | 4.76 | – |

### 3–3. Investigating pseudo Juan–Teller effect on distortion of analog containing As 1,3–di(pyridine–2–yl) Benzonium atom (compound No. 3)

As it was mentioned in previous structures, the structure of compound No. 3 has C2V high symmetry, and has low symmetry in point group. Deviations are the result of combining the compound of ground state A1 and excited level B2 by displacement b2, as well as the result of combining the ground state A1 and excited level B1 through displacement b1. Combination of excited level B2 with excited level B1 and combination of excited level A2 with excited level A1 is done through displacement a2. (It has to be noted that in the third case, the ground state cannot combine with excited states as it is aligned with them, so it doesn't create psuedo Juan-Teller effect, and devations with the combination of non-aligned excited levels results in creation of psuedo Juan-Teller effect.) Here, the pseudo Juan-Teller results in (A1+B2) ⊗ b2, (A1+B1) ⊗ b1, (B2+B1) ⊗ a2, and (A2+A1) ⊗ a2 problems.



FIGURE 8. Symmetrical transformation of C2V of analog containing As 1,3-di(pyridine-2-yl) Benzonium atoms in form of Cs (C2V → Cs) using calculations in B3LYP/6-311++G** theoretical level

Figures 9, 10, and 11 show the energy of ground level and excited levels, as well as the deviations of arrangements with high symmetry due to pseudo Juan-Teller effect. The energy difference between ground level and excited level B2 (first case), shown in Figure 9, and between ground level and excited level B1 (second case), shown in Figure 10, and between a pair of excited levels of B2 and B1 and another pair of excited levels of A2 and A1 (third case), shown in Figure 11, along with the combination of orbitals is 3.50, 3.78, and 0.03-0.25 eV, respectively.

1. [Homo – 4 (B2) → Lumo + 2 (A1), Homo – 1(B1) → Lumo+1(A2)]
2. [Homo – 1 (B1) → Lumo + 2 (A2)]
3. [Homo – 4 (B2) → Lumo (B1), Homo (A2) – Lumo +2 (A1), Homo → 3(B1) – Lumo (B1), Homo (A2) – Lumo + 1(A2), Homo (A2) – Lumo + 3 (A2), Homo → 4 (B2) – Lumo + 2(A1), Homo → 1(B1) – Lumo + 1 (A2), Homo → 1(B1) – Lumo + 2 (A1)]
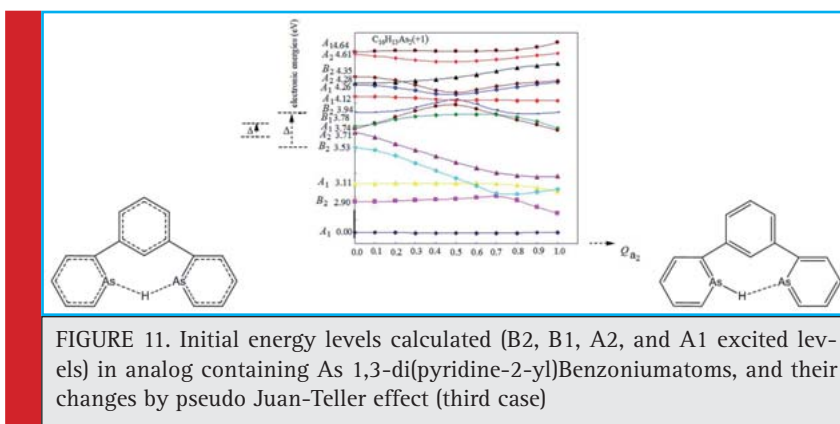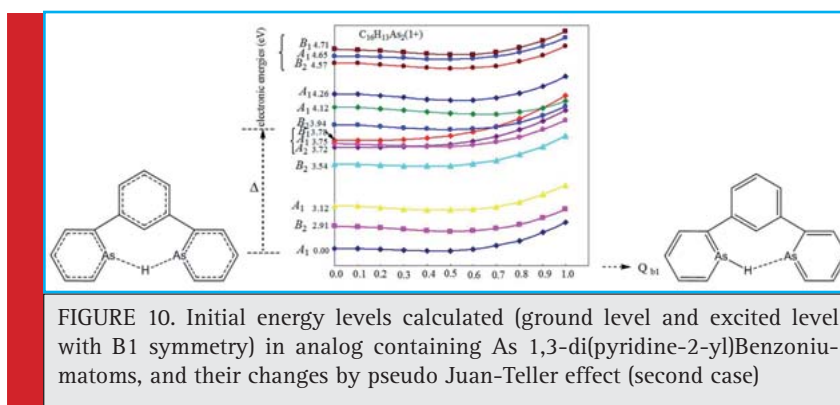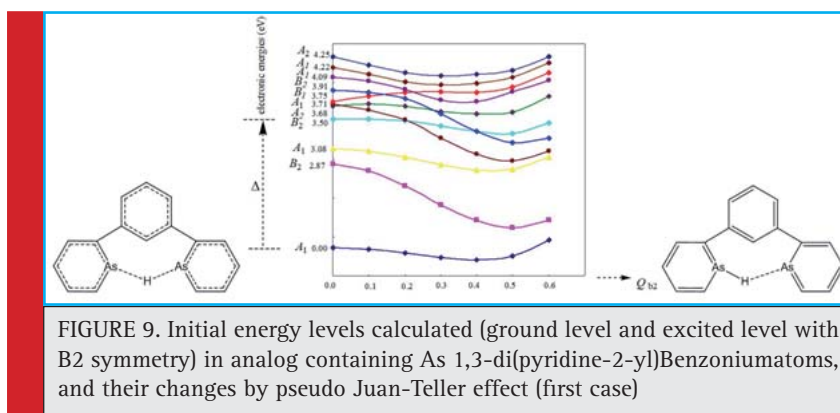
Comparison between the first and second case shows that according to the reduction in energy difference in the first case, its pseudo Juan-Teller energy is higher, and comparison between the three cases indicates that the pseudo Juan-Teller of the third case is the highest (in case just one single factor of energy difference between ground level and excited level (Δ) is considered).

The electron energy of a number of excited levels for the structure No. 3, calculated in B3LYP/6-311++G** theoretical level (eV), is reported in Table 4. It shows that the excited level B2 with an approximate energy of 3.50 eV (first case), and the excited level B1 with an approxi-

FIGURE 9. Initial energy levels calculated (ground level and excited level with B2 symmetry) in analog containing As 1,3-di(pyridine-2-yl)Benzoniumatoms, and their changes by pseudo Juan-Teller effect (first case)



FIGURE 10. Initial energy levels calculated (ground level and excited level with B1 symmetry) in analog containing As 1,3-di(pyridine-2-yl)Benzoniumatoms, and their changes by pseudo Juan-Teller effect (second case)



FIGURE 11. Initial energy levels calculated (B2, B1, A2, and A1 excited levels) in analog containing As 1,3-di(pyridine-2-yl)Benzoniumatoms, and their changes by pseudo Juan-Teller effect (third case)

mate energy of 3.78 eV (first case) contribute in creating pseudo Juan-Teller effect.

The value of thermodynamic parameters $\Delta G$, $\Delta H$, $\Delta S$, and $\Delta Ee1$ of the desired compound, shown in Table 2, was calculated using B3LYP/6-311++G** method.

The results show that the value of $\Delta Ee1$ for the compound No. 3 is 21.74 kCal/mol, 11.87 kCal/mol, and 1.06 kCal/mol for the first, second, and third case, respectively, which implies that the desired compound in the third state has lower pseudo Juan-Teller stability energy.

The results of B3LYP/6-311++G** calculations for the three compound 1, 2, and 3 show that the major

cause of deformation of configurations with C2V high symmetry to Cs low symmetry configurations is pseudo Juan-Teller effect. The energy difference ($\Delta$) between the reference states from compound 1 to compound 3 (i.e., 5-35-5.55 eV, 4.46-5.10 3 eV, and 0.03-0.25-3.5-3.78 eV for compounds 1, 2, and 3, respectively) decreases. So, it is expected that the pseudo Juan-Teller energy for these deformations (C2V → Cs) increases from compound (1) to (3). The results obtained bu applying this method to determine the energy of the ground state from compound (1) to (3) for B2 symmetry (79.02, 27.97, and 21.74 kcal-mol-1 for compound 4, 5, and 6, respectively) and for

Table 4. Investigating the energy of excited levels (eV) of C2V analog containing As 1,3-di(pyridine-2-yl)Benzonium atoms with symmetrical arrangement (C2V → Cs) (three cases).

| | $B_2$ | $A_1$ | $B_2$ | $A_2$ | $A_1$ | $B_1$ |
|---|---|---|---|---|---|---|
| 1. $C_{16}H_{13}As_2(+1)$ | 2.87 | 3.08 | 3.50 | 3.68 | 3.71 | 3.75 |
| 2. $C_{16}H_{13}As_2(+1)$ | 2.91 | 3.12 | 3.53 | 3.72 | 3.75 | 3.78 |
| 3. $C_{16}H_{13}As_2(+1)$ | 2.90 | 3.11 | 3.53 | 3.71 | 3.74 | 3.78 |

B1 symmetry (48.01, 15.35, and 11.78 21.74 kcalmol-1 for compound 1, 2, and 3, respectively) decreases, which implies that the compound (1) has the highest pseudo Juan-Teller stability energy.

## CONCLUSION

The results obtained by calculations in B3LYP/6–311++G** theoretical level shows that the pseudo Juan-Teller effect explains C2V high symmetry structural deformation to Cs low symmetry structure in the following compounds:

1,3-di(pyridine-2-yl)Benzonium (compound 1)
Analog containing P 1,3-di(pyridine-2-yl)Benzonium atom (compound 2)
Analog containing As 1,3-di(pyridine-2-yl)Benzonium atom (compound 3)

It was found that the hydrogen bond of compounds (1) to (3) have C2V high symmetry configuration.

By Q transformations, the first three compounds (1 to 3) transform from C2V high symmetry base configuration to Cs low symmetry excited configuration. It is associated with decreasing the electron energy of ground state electron configurations and increasing the electron energy of excited state electron configurations. This study addressed the mixing of electron ground state with electron excited states in the direction of applying normal coordination, describing leaving high symmetry and transforming into low symmetry. Therefore, the distortion of C2V high symmetry having hydrogen bond in compounds (1)-(3) is due to pseudo Juan-Teller effect (PJTE), (A1+B2) ⊗ b2, and (A1+B1) ⊗ b1, which is created by combining the ground state and excited states. It has to be noted that meanwhile, the energy difference (ΔE) between reference states from compound (1) to (3) (i.e., 5.33-5.5 eV, 4.46-5.10 eV, 0.03-0.25-3.5-3.78 eV for 1,3-di(pyridine-2-yl)Benzonium, analog containing P atom, and analog containing As atom, respectively) decreases. Furthermore, examining pseudo Juan-Teller for these deformations (C2V → Cs) showed that the pseudo Juan-Teller stability energy decreases from compounds (1) to (3).

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