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# Investigation on Molecular Structure and Electronic Properties of Zinc (II) Complex with 2-acetylpyridinenicotinichydrazone Ligand

**Guventurk UGURLU**
Kafkas University

**Ahmet HARMANKAYA**
Kafkas University

**Abstract:** In the present study, the structural parameter, the electronic and nonlinear optical properties of three Zn (II) halido complexes of the type [Zn (Hal)2HL] (Hal = Cl, **1**; Br, **2**; I, **3**; HL = 2-acetylpyridine nicotinic hydrazone) have been theoretically investigated in detail. Two of the studied complexes [ZnCl2(HL), [ZnBr2(HL)] have been synthesized before, and some molecular properties have been determined, however, the new complex [ZnI2(HL)] is theoretically modeled for the first time. The polarizability (α), dipole moment (μ) and the first-order hyperpolarizability (β) of the compounds have been investigated using the Density Functional Theory (DFT) based on the B3LYP density functional with basis set combinations. In calculations, LANL2DZ and a mixed basis set of LANL2DZ (for Zn and I) and 6-311G (for other atoms) are used in the gas-phase geometry optimization. In addition, the highest occupied molecular orbital energy (HOMO) and the lowest unoccupied molecular orbital (LUMO) of the compounds in the ground state were calculated by using the same method and the energy band gap (Eg = $E_{LUMO}$-$E_{HOMO}$) was obtained from frontier molecular orbitals. The equilibrium state (ground state) dipole moment value of the studied complex was calculated as 12.61 and 12.74 Debye by B3LYP/GENECP/LANL2DZ-6-311G and B3LYP/LANL2DZ method, respectively. The energy gap values of complexes **1-3** are calculated as 1.73/1.38/1.15 eV at the B3LYP/LANL2DZ and are calculated as 3.61/2.28/2.18 eV at the B3LYP/MIX respectively. The energy gap values of complexes **1-3** decrease in the order complex 1>complex 2>complex 3. The approximate geometry of the molecules in three dimensions was drawn in the Gauss View 5.0 molecular imaging program, and all theoretical calculations were used with the Gaussian 09W package program.

**Keywords:** B3LYP/GENECP/LANL2DZ-6-311G, Dipole moment, Polarizability, Hyper polarizability, 2-acetylpyridine nicotinic hydrazone

## Introduction

The development of new heterocyclic organic compounds has received considerable attention due to their potential fluorescence applications, theoretical properties, biological or ionic probes and lighting Technologies. (Bahçeci et al., 2016; Kardaş et al., 2016; Bahçeci et al., 2017; Aktaş Yokuş et al., 2017; Çiftçi et al., 2018; Beytur et al., 2019; Beytur et al., 2019; Irak & Beytur, 2019; Kotan et al., 2020; Uğurlu, 2020; Uğurlu & Beytur, 2020; Beytur, 2020; Koç et al., 2020; Beytur & Avinca, 2021; Boy et al, 2021). The metal-organic supramolecular systems continue to attract the attention of researchers because of their potential applications as functional materials in various fields (Xu et al., 2017; Sertçelik, 2020; Sertçelik & Durman, 2020). Acyl-hydrazone having different heteroatoms in its structure is used as ligands in coordination chemistry as polydentate ligands for the synthesis of metal complexes (Santiago et al., 2020). Metal complexes based on Schiff bases are frequently used in coordination chemistry and the widening of application areas increases their importance (Reddy et al., 2016; Gönül et al., 2016; Al-Humaidi et al., 2019). Scientific studies on these compounds continue to increase due to their pharmacological properties (Xiao et al., 2004; Naskar et al., 2007; Dash et al., 2012; Sutradhar et al., 2013). Compounds, $ZnCl_2$(HL) and [$ZnBr_2$(HL) were synthesized in 2020

and some molecular properties were determined (Santiago et al., 2020). The complex [$ZnI_2$(HL)] was theoretically modeled for the first time in this study. The α, μ, β, HOMO and LUMO values of the complexes **1-3** and HL molecule have been investigated theoretically by using B3LYP/GENECP/LANL2DZ-6-311G and B3LYP/LANL2DZ methods. The energy values of all three complex compounds were calculated and compared with the experimental values in the literature. One of the objectives of this study is to determine the metal coordination ability of HL. So, the negative area (red area) and the positive area (blue area) on the MESP of HL have been calculated and discussed. The atomic numbering scheme of the compounds is given in Figure 1.

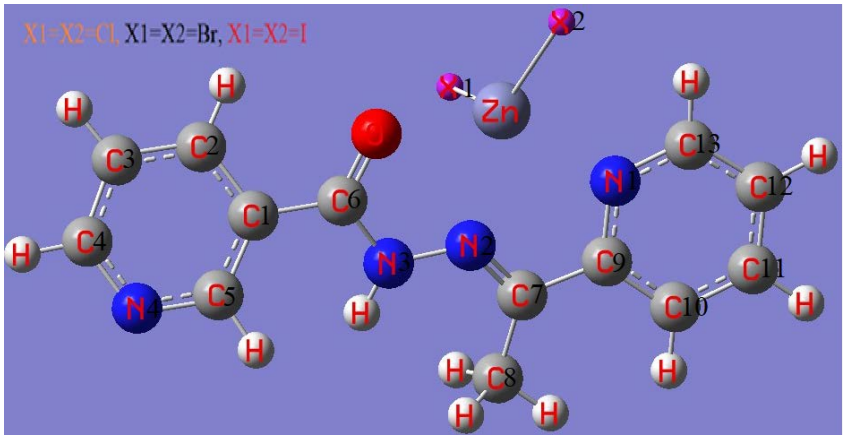


Figure 1. The theoretical geometric structure of the compounds

## Methods

Firstly, geometry optimizations of complexes **1-3** and HL in the ground state have been performed using both B3LYP/GENECP/LANL2DZ-6-311G and B3LYP/LANL2DZ methods after optimization calculations, optimized structure obtained have been used to calculate the properties of these compounds. Computations were done with Gaussian 09 (Frisch et al., 2010) and Gauss view 5.0.9 (Dennington et al., 2009) software using Density Functional Theory (DFT) ( Kohn et al., 1965) with B3LYP; Becke's three parameters exact exchange functional (B3) combined with the gradient corrected correlation functional of Lee–Yang–Parr (LYP) (Becke et al., 1988; Lee et al., 1988; Becke, 1993) methods by implementing LANL2DZ and a mixed basis set of LANL2DZ (Rappe et al., 1992) (for Zn and I) and 6-311G (for other atoms). The potential map electrostatic surface (MESP) of HL and the frontier orbitals (HOMO-Highest Occupied Molecular Orbital), (LUMO-Lowest Unoccupied Molecular Orbital) of all the compounds have been calculated by the same methods. The energy gap (Eg) values of the compounds studied have been obtained by using HOMO-LUMO energies utilizing the following equation.

$Eg = E_{LUMO} - E_{HOMO}$

## Results and Discussion

### Geometrical Structure

The geometry optimization structures of compounds obtained by B3LYP/LANL2DZ and B3LYP/GENECP/LANL2DZ-6-311G (B3LYP/MIX) methods, respectively are compiled and are tabulated in Table 1. The MESP of HL and optimized structures of complexes **1-3** are given in Figure 2. As seen in Figure 2. The zinc (II) metal is attached to 2-acetylpyridine nicotinic hydrazone molecule and two halogen atoms such as iodine, bromine, and chlorine. Since the complexes molecular structures of the studied **1-3** are not available in the literature, the calculated values of the structural parameters were compared with the parameters of molecules with similar structures (Santiago et al., 2020). As seen from Table 1. in the complexes, at the B3LYP/LANL2DZ, X1-Zn bond length is calculated as 2.3454/2.5198/2.713 Å (complex **1**/complex **2**/complex **3**) and at the B3LYP/MIX, calculated as 2.3629/2.4980/2.7129 Å (complex **1**/complex **2**/complex **3**) respectively. Similarly, in the complex, at the B3LYP/LANL2DZ, X2-Zn bond length is calculated as 2.3104/2.4752/2.6741 Å (complex **1**/complex **2**/complex **3**) and at the B3LYP/MIX, calculated as 2.3232/2.4557/2.6687 Å (complex **1**/complex **2**/complex **3**) respectively. As can be seen from these values, the X1-Zn bond has a higher value than the X1-Zn bond at both methods and is consistent with the experimental

value. Also, the Zn-O bond length is calculated as 2.2653/2.2646/2.2442 Å at theB3LYP/LANL2DZ and is calculated as 2.2635/2.2824/2.2825 Å (complex **1**/complex **2**/complex **3**) at the B3LYP/MIX respectively. The calculated values of the electronic, dipole moment, polarizability, hyperpolarizability, HOMO, LUMO energy and energy gap (Eg) at the ground-state equilibrium geometry of studied molecules are listed in Table 2. The dipole moment value of the molecule was calculated as 5.43 Debye by the B3LYP/6-311++G(2d,2p) method and as 5.73 Debye by the HF/6-311++G(2d,2p) method, respectively.

Table 1. The bond lengths and angles of the complexes, GENECP/LANL2DZ-6-311G abbreviated as MIX.

| | | | Bond length (Å) | | | | |
|---|---|---|---|---|---|---|---|
| Atoms | | B3LYP/LANL2DZ | | | B3LYP/ /MIX. | | |
| | Exp[a] | X1=X2=Cl | X1=X2=Br | X1=X2=I | X1=X2=Cl | X1=X2=Br | X1=X2=I |
| X1-Zn | 2.698(3) | 2.3454 | 2.5198 | 2.7183 | 2.3629 | 2.498 | 2.7129 |
| X2-Zn | 2.365(3) | 2.3104 | 2.4752 | 2.6741 | 2.3232 | 2.4557 | 2.6687 |
| Zn-O | 2.015(3) | 2.2653 | 2.2646 | 2.2442 | 2.2635 | 2.2824 | 2.2825 |
| Zn-N1 | 2.037(3) | 2.2249 | 2.2322 | 2.2294 | 2.235 | 2.2454 | 2.2491 |
| Zn-N2 | 1.930(3) | 2.2591 | 2.2511 | 2.2602 | 2.2574 | 2.2605 | 2.2534 |
| O-C6 | 1.282(4) | 1.2596 | 1.2597 | 1.26 | 1.2533 | 1.2526 | 1.2526 |
| N1-C9 | -- | 1.3675 | 1.3681 | 1.3667 | 1.3623 | 1.3622 | 1.3625 |
| N1-C13 | -- | 1.3482 | 1.3483 | 1.349 | 1.3429 | 1.343 | 1.3432 |
| N2-N3 | -- | 1.3742 | 1.3752 | 1.3755 | 1.3688 | 1.3694 | 1.3703 |
| N2-C7 | 1.284(5) | 1.3043 | 1.3053 | 1.305 | 1.2966 | 1.2975 | 1.2991 |
| N3-C6 | 1.320(5) | 1.3969 | 1.3963 | 1.3955 | 1.388 | 1.3877 | 1.3874 |
| N4-C5 | -- | 1.3532 | 1.353 | 1.3528 | 1.3458 | 1.3458 | 1.3456 |
| N4-C4 | -- | 1.3583 | 1.3584 | 1.3584 | 1.3522 | 1.3522 | 1.3522 |
| C6-C1 | -- | 1.4825 | 1.4822 | 1.4822 | 1.4736 | 1.4741 | 1.4741 |
| C7-C9 | -- | 1.491 | 1.4895 | 1.4892 | 1.4837 | 1.4821 | 1.4812 |
| C7-C8 | -- | 1.5113 | 1.5113 | 1.5116 | 1.5025 | 1.5025 | 1.503 |
| C7-C10 | -- | 1.4076 | 1.408 | 1.4085 | 1.3975 | 1.3979 | 1.3986 |
| C1-C5 | -- | 1.4138 | 1.414 | 1.4141 | 1.4027 | 1.4028 | 1.4028 |
| C1-C2 | -- | 1.4129 | 1.413 | 1.4132 | 1.4039 | 1.4038 | 1.4041 |
| C10-C11 | -- | 1.4089 | 1.4084 | 1.4074 | 1.3984 | 1.3981 | 1.3975 |
| C2-C3 | -- | 1.4021 | 1.4021 | 1.402 | 1.3916 | 1.3917 | 1.3916 |
| C12-C11 | -- | 1.4039 | 1.4039 | 1.4047 | 1.3923 | 1.3926 | 1.393 |
| C4-C3 | -- | 1.4098 | 1.4098 | 1.4097 | 1.397 | 1.397 | 1.397 |
| | | | | Bond angle (˚) | | | |
| X1-Zn-X2 | 103.09(2) | 130.8 | 131.4 | 132.1 | 133.2 | 131.8 | 132.5 |
| X1-Zn-0 | 97.22(8) | 94.3 | 94.9 | 96.1 | 94.4 | 95.1 | 96.2 |
| X1-Zn-N1 | 93.88(9) | 101.0 | 99.6 | 97.5 | 99.3 | 99.6 | 98.0 |
| X1-Zn-N2 | 95.23(10) | 90.9 | 92.9 | 97.9 | 91.5 | 93.6 | 97.7 |
| X2-Zn-0 | | 102.8 | 101.3 | 99.1 | 102.2 | 101.4 | 99.5 |
| X2-Zn-N1 | | 96.1 | 97.2 | 98.4 | 96.2 | 97.2 | 98.2 |
| X2-Zn-N2 | 161.68(10) | 138.2 | 135.7 | 129.9 | 135.2 | 134.6 | 129.8 |
| O-Zn-N1 | 156.70(12) | 138.2 | 139.2 | 141.1 | 138.8 | 138.5 | 139.8 |
| O-Zn-N2 | 79.33(12) | 70.2 | 70.4 | 70.7 | 70.3 | 70.0 | 70.2 |
| N1-Zn-N2 | 79.31(13) | 70.8 | 71.0 | 71.4 | 70.7 | 70.5 | 70.7 |
| Zn-O-C6 | | 116.2 | 116.8 | 118.2 | 116.4 | 116.5 | 117.2 |
| Zn-N1-C9 | | 117.8 | 117.7 | 117.6 | 117.6 | 117.7 | 117.6 |
| Zn-N1-C13 | | 121.6 | 121.8 | 122.2 | 121.8 | 121.8 | 121.9 |
| C9-N1-C13 | | 120.4 | 120.2 | 120.0 | 120.4 | 120.3 | 120.3 |
| Zn-N2-N3 | | 114.5 | 115.0 | 115.1 | 114.4 | 114.9 | 115.6 |
| Zn-N2-C7 | | 119.3 | 120.0 | 120.0 | 119.7 | 120.0 | 120.6 |
| N3-N2-C7 | | 123.2 | 123.0 | 124.0 | 123.4 | 123.1 | 122.9 |
| N2-N3-C6 | | 115.0 | 115.1 | 115.4 | 115.5 | 115.7 | 115.9 |
| O-C6-N3 | | 119.6 | 119.4 | 119.3 | 119.7 | 119.7 | 119.6 |
| O-C6-C1 | | 122.7 | 122.7 | 122.5 | 122.6 | 122.7 | 122.6 |
| N3-C6-C1 | | 117.8 | 117.9 | 118.2 | 117.7 | 117.6 | 117.8 |

([a])taken from Santiago et al. (2020)

X1-Zn-X2 bond angle is calculated 130.8/131.4/132.1˚ at the B3LYP/LANL2DZ and is calculated 133.2/131.8/132.5˚ (complex 1/complex 2/complex 3) at the B3LYP/MIX respectively. N1-Zn-N2 bond angle is

calculated 70.8/71.0/71.4° at theB3LYP/LANL2DZ and is calculated 70.7/70.5/70.7° (complex **1**/complex **2**/complex **3**) at the B3LYP/MIX respectively. The corresponding experimental value in the literature [3] is 79.31°. The color code of HL lies in the range of $-8.349e^{-3}$ to $+8.349e^{-3}$. Red and blue colors on the MEP surface indicate electron-rich and electron-poor regions, respectively (Scrocco et al., 1978; Arjunan et al., 2011). The MEP of HL has many possible sites for electrophilic (presented in red color) and nucleophilic attack (presented by as blue color). In the optimized structures of complexes **1-3,** it is seen that Zn is located in the region with the most pronounced negative potential.

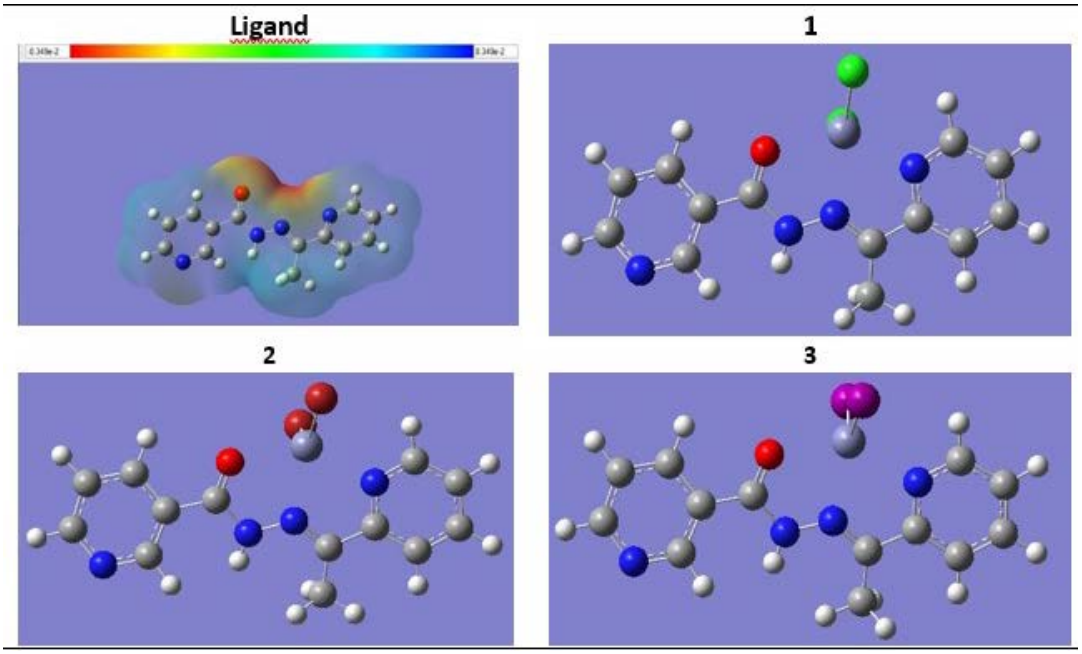


Figure 2. MESP of HL and optimized structures of complexes **1-3**

The dipole moment, polarizability, hyperpolarizability, HOMO and LUMO values of the complexes 1-3 and the HL molecule have been calculated by using the B3LYP/GENECP/LANL2DZ-6-311G and B3LYP/LANL2DZ methods and these values are presented Table 2.

Table 2. HOMO, LUMO energy, dipole moment, polarizability, hyperpolarizability, and energy gap ($E_g$) of the compounds

| B3LYP/LANL2DZ | | | | | | |
|---|---|---|---|---|---|---|
| Compound | μ (D) | α (a.u) | β(a.u) | $E_{HOMO}$ (a.u) | $E_{LUMO}$ (a.u) | $E_g$ (eV) |
| Complex 1 | 21.96 | 268.7 | 10448.4 | -0.182486 | -0.119089 | 1.73 |
| Complex 2 | 22.78 | 286.9 | 10862.2 | -0.17192 | -0.12105 | 1.38 |
| Complex 3 | 22.72 | 314.5 | 13261.5 | -0.164676 | -0.122422 | 1.15 |
| Ligand | 4.79 | 201.5 | 173.7 | -0.244216 | -0.074594 | 4.62 |
| B3LYP/GENECP/LANL2DZ-6-311G/MIX | | | | | | |
| Complex 1 | 12.28 | 221.9 | 1300.1 | -0.239171 | -0.123047 | 3.16 |
| Complex 2 | 12.28 | 235.1 | 1996.2 | -0.221215 | -0.122667 | 2.68 |
| Complex 3 | 12.61 | 253.5 | 3969.7 | -0.204503 | -0.124471 | 2.18 |

The energy gap ($E_g$) between frontier orbitals describes a significant stability factor, and $E_g$ helps to determine the chemical reactivity and kinetic stability of the compounds (Ramamoorhyet al., 2017; Ramya et al., 2017; Ramya et al., 2017). The energy gap values of complexes **1-3** are calculated as 1.73/1.38/1.15 eV at the B3LYP/LANL2DZ and are calculated as 3.61/2.28/2.18 eV at the B3LYP/MIX respectively. The energy gap values of complexes **1-3** decrease in the order complex **1**>complex **2**>complex **3**. The change in the hyperpolarizability values of the **1-3** complexes is the inverse of the change in energy gap values. That is, the hyperpolarizability values of complexes **1-3** increase in order: complex **1**<complex **2**<complex **3**.

**Frontier Molecular Orbitals**

Frontier molecular orbitals and their features like energy are important to physicists and chemists. The HOMO represents the electron donor and LUMO (lowest occupied molecular orbital) represents the electron acceptor. The HOMO and LUMO plots of all the compounds are shown in Figure 3. As seen in the figure.3, the frontier molecular orbital LUMO of all the compounds have exhibited similar behavior and the charge density has localized all over the entire of each compound. The frontier molecular orbital HOMO of complexes **1-3** have exhibited similar behavior and the charge density has localized in the region of the zinc atom. The frontier molecular orbital HOMO of HL shows the charge density localized all over the molecule except for the nicotinic ring.

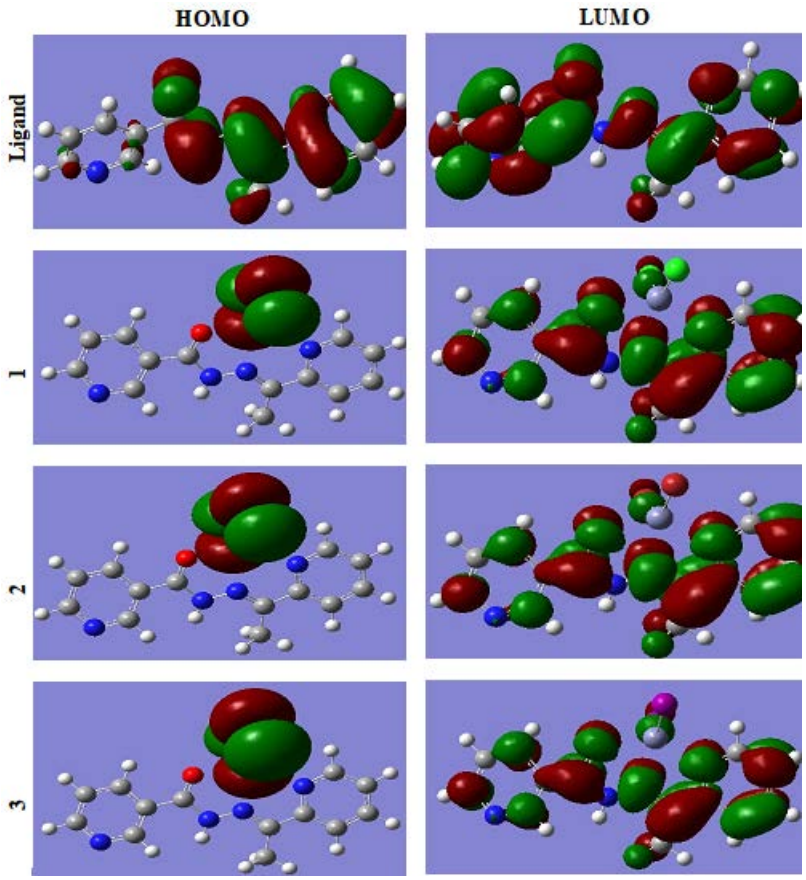


Figure 3. The shapes of the HOMO-LUMO orbitals of complexes **1-3** and HL at the B3LYP/MIX

## Conclusions

In this work, the lowest unoccupied molecular orbital (LUMO) and the highest occupied molecular orbital (HOMO), structural parameters, dipole moments and nonlinear optical properties of complexes **1-3** and HL were calculated by both B3LYP/LANL2DZ and B3LYP/GENECP/LANL2DZ-6-311G (B3LYP/MIX) methods. In the optimized structures of complexes **1-3,** it is seen that Zn is located in the region with the most pronounced negative potential. The frontier molecular orbital HOMO of complexes **1-3** have exhibited similar behavior and the charge density has localized in the region of the zinc atom. The order of the energy gap values of complexes **1-3** is complex **1**>complex **2**>complex **3**. The change in the hyperpolarizability values of the **1-3** complexes is the inverse of the change in energy gap values. That is, the hyperpolarizability values of complexes **1-3** increase in order: complex **1**<complex **2**<complex **3**.

## Scientific Ethics Declaration

The authors declare that the scientific ethical and legal responsibility of this article published in EPSTEM journal belongs to the authors.

## Acknowledgements or Notes

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## Author Information

**Guventurk Ugurlu**
Kafkas University
Kars,Turkey
Contact E- mail:*gugurlu@kafkas.edu.tr*

**Ahmet Harmankaya**
Kafkas University
Kars,Turkey

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