The Molecular Structure and Spectral Characteristics of Heavy Metal Chelating Agent of H₃TMT and Its Complex (HgMe)₃TMT with CH₃HgCl

Feng-Yun Wang, Feng-He Wang, and Xue-Dong Gong

Abstract—In order to explore the molecular structure and spectral characteristics of 2,4,6-trimercaptotriazine (H₃TMT) and its heavy metal chelating complex (HgCH₃)₃TMT, quantum chemical calculations were performed using the density functional theory, B3LYP method. With the optimized geometries of H₃TMT and (HgCH₃)₃TMT, ¹³C NMR chemical shifts and IR spectroscopic characteristics were calculated. In order to describe the molecular characteristics more accurately, descriptors such as the frontier molecular orbital energy, Fukui indices, the natural population analysis and global reactivity were obtained. In combination with the compositions of the highest orbital molecular orbital (HOMO), and the local reactivity descriptors, S and N atoms in H₃TMT are the reactive sites, as was seen in the formation of metal complex of (HgCH₃)₃TMT with CH₃HgCl. The calculated molecular geometries, ¹³C NMR chemical shifts and IR spectroscopic characteristics of (HgCH₃)₃TMT are in good agreement with the experimental results, which indicates the simulation is reasonable. Theoretical investigation upon the heavy metal chelating agent of H₃TMT is undoubtedly helpful for the design and synthesis of new materials, as well as the assessment of material performance.

Index Terms—Density functional theory, quantum chemistry, 2,4,6-trimercaptotriazine (H₃TMT), heavy metal chelating agent.

I. INTRODUCTION

Due to the toxicity to human life and the environment, pollution of heavy metals becomes one of the most important worldwide ecological problems. During last decades, heavy metals have been largely introduced into the environment from natural and anthropogenic sources [1]. Among heavy metals, mercury is the second most toxic metal [2], and is also classified as the priority pollutant by the US Environmental Protection Agency (USEPA) [3]. Generally, mercury occurs in the environment as metallic, inorganic or organic mercury, and its ecological and toxicological effects are strongly dependent on its chemical form [4], [5]. Inorganic mercury has been reported to produce harmful effects at the concentration as low as 5 µg/L [6], but organomercury compounds can exert the same effect at the concentration 10

times lower [7]. That is to say, the organic Hg compound is more toxic to living organisms than the inorganic ones [8]. Inorganic mercury can be converted into methyl mercury by methanogenic bacteria in aquatic environments [1], which is water-soluble. The lipophilic nature of methylmercury results in much more bioaccumulation in the aquatic food chain [9], and the up-level transfer to reach human diet [10]. Methylmercury triggers several serious disorders for humans including allergic reactions and brain and neurological damages [11], and it can cause chronic and acute human mercury poisoning such as Minamata disease [12]. Therefore, the elimination of methylmercury from water and wastewater is important to protect public health, and have received considerable attentions [13].

2, 4, 6-trimercaptotriazine (trithiocyanuric acid, C₃H₃N₃S₃, denoted further as H₃TMT) and its trisodium salt (TMT) have lower toxicity for organism [14]. Owing to the role of three N and S donors, it displays a great versatility of coordination with transition metals, and has been practiced for precipitating divalent and univalent heavy metals to immobilize these heavy metals in soil for in situ remediation [15]. Studies have been reported that H₃TMT and TMT can precipitate CH₃HgCl directly for their powerful complexing capability [15], the main group and transition metal TMT compounds have steady chemical property, and show good stability in environment, which can avoid the secondary pollution in the process of heavy metal pollution control by using TMT. In spite of extensive research efforts with H₃TMT and TMT, our knowledge of the mechanism of TMT reactions remains limited, except for a few information on how the product reacts with heavy metals in aqueous solutions, and the chemistry and stability of the resulting heavy metal TMT precipitates. Since the molecular geometries and electronic structures are the foundations for the study of structure-performance relations, in the current study, systematic theoretical investigations on the formation process and the stability mechanism of (HgCH₃)₃TMT were investigated at the molecular level with density functional theory method (DFT). Based on the optimized geometries of H₃TMT and (HgCH₃)₃TMT, the information about the molecular orbitals energy levels, natural atomic charges, vibration frequencies, and Fukui indices etc. were provided, and a comparison was made between the information obtained from calculations in this study and that reported previously in the literature. It is hopeful that findings of this study will help us to establish the structure-performance relationships, and to better understand how H₃TMT is activated and further interacts with transition metal centers.

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II. COMPUTATIONAL METHOD

Many studies have shown that the DFT-B3LYP method in combination with the 6-31++G(d,p) basis set is able to give accurate energies, structures, and vibrational frequencies [16]. It is also employed in this paper, and for Hg for which the 6-31++G(d,p) basis set is not available, the pseudo potential basis set of SDD is used. All computations were performed using the Gaussian 03 software package [17] without any priori symmetry restriction and with default thresholds on residual forces and displacements. After optimization, the analyses of harmonic vibrational frequencies were performed at the same level, which was considered as a guarantee of energetically minimum point on the potential surface.

III. RESULTS AND DISCUSSIONS

A. Molecular Geometries

The fully optimized molecular geometries of H_3TMT and $(\text{HgCH}_3)_3\text{TMT}$ were shown in Fig. 1.

Fig. 1. Optimized geometries of H_3TMT and $(\text{HgCH}_3)_3\text{TMT}$.

TABLE I: SELECTED BOND LENGTHS (Å) FOR H_3TMT AND $(\text{HgCH}_3)_3\text{TMT}$

Bond lengths	$(\text{HgCH}_3)_3\text{TMT}$		H_3TMT	
	Exp.	Theory	Error/%	Theory
Hg(10)–C(13)	2.13	2.11	-0.90	
Hg(10)–S(7)	2.37	2.45	3.15	
Hg(11)–C(14)	2.06	2.12	2.48	
Hg(11)–S(8)	2.40	2.45	2.31	
Hg(12)–C(15)	2.10	2.11	0.95	
Hg(12)–S(9)	2.38	2.45	2.75	
S(7)–C(1)	1.67	1.76	5.02	1.76
S(8)–C(3)	1.74	1.76	0.86	1.76
S(9)–C(5)	1.65	1.76	6.35	1.76
N6–C5	1.31	1.34	2.06	1.34
N6–C1	1.38	1.35	-2.49	1.34
N2–C3	1.34	1.35	0.50	1.34
N2–C1	1.37	1.34	-2.40	1.34
N4–C3	1.24	1.34	7.80	1.34
N4–C5	1.48	1.35	-8.50	1.34
Hg(10)–N(6)	2.82	2.89	2.53	
Hg(11)–N(2)	2.87	2.89	0.93	
Hg(12)–N(4)	2.84	2.90	2.10	

As can be seen in Fig. 1, Hg of HgCH_3 binds with S in an

almost straight line, H_3TMT and $(\text{HgCH}_3)_3\text{TMT}$ have approximately C_3 symmetrical structure. Some key geometrical parameters are collected in Table I and Table II. Among the studied systems, only $(\text{HgCH}_3)_3\text{TMT}$ has experimental X-ray single crystal structure [15], which is also listed in Table I and Table II for comparison.

TABLE II: SELECTED BOND ANGLES (°) FOR H_3TMT AND $(\text{HgCH}_3)_3\text{TMT}$

Bond angles	$(\text{HgCH}_3)_3\text{TMT}$			H_3TMT
	Exp.	Theory	Error/%	Theory
C(13)–Hg(10)–S(7)	178.2	177.75	-0.26	
C(14)–Hg(11)–S(8)	173.7	177.74	2.31	
C(15)–Hg(12)–S(9)	174.8	177.62	1.61	
C(1)–S(7)–Hg(10)	93.8	94.96	1.22	
C(3)–S(8)–Hg(11)	96.5	94.97	-1.60	
C(5)–S(9)–Hg(12)	95.8	95.0	-0.85	
C5–N6–C1	124.3	124.52	0.18	114.04
C3–N2–C1	117.3	115.47	-1.56	114.04
C3–N4–C5	115.3	115.47	0.15	114.05
N2–C1–N6	116.3	115.49	-0.70	125.96
N2–C1–S7	120.3	117.17	-2.60	115.16
N6–C1–S7	122.3	118.31	-3.26	118.88
N4–C3–N2	130.3	124.54	-4.42	125.95
N4–C3–S8	113.2	117.14	3.48	115.16
N2–C3–S8	117.2	118.32	0.96	118.89
N6–C5–N4	117.3	124.52	6.15	125.96
N6–C5–S9	123.3	117.13	-5.00	115.18
N4–C5–S9	120.3	118.35	-1.62	118.86

The theoretical results match the experimental results well for $(\text{HgCH}_3)_3\text{TMT}$ [15], which indicates that the theoretical method is reliable. Covalent radius of N, S and Hg is 0.75 Å, 1.02 Å and 1.49 Å respectively [18]. As observed in Fig. 1, the bond lengths of Hg(10)–N(6), Hg(11)–N(2) and Hg(12)–N(4) is 2.82 Å, 2.87 Å and 2.84 Å respectively, which is a bit longer than its covalent bond length of 2.24 Å, indicating a weak bond of Hg–N was formed. Cecconi [15] surmised that there remained a secondary action between Hg · N, and conjectured the bond length of Hg · N was 2.82(3)~2.87(3) Å, which is in agreement with the computing results. The bond lengths of S(7)–C(1), S(8)–C(3) and S(9)–C(5) in $(\text{HgCH}_3)_3\text{TMT}$ are shorter than that in H_3TMT , the bond length of S–C is shorter than the normal length, which indicates a delocalization in the conjugated system

B. The Frontier Molecular Orbitals

It is essential to examine frontier orbitals owing to their close relationship with the excitation properties and active sites involving a coordinatively unsaturated transition metal center [19]. The highest occupied molecular orbitals (HOMO) and the lowest unoccupied molecular orbitals (LUMO) transition is the leading electron configuration for the first excited state, thus, the lowest lying singlet excited state for H_3TMT comprises mainly an electronic transition from HOMO to LUMO. Compositions of HOMO and LUMO of H_3TMT and contributions of atoms are shown in Table III.

TABLE III: COMPOSITIONS OF HOMO AND LUMO OF H₃TMT AND CONTRIBUTIONS OF ATOMS

Item	C1	N2	C3	N4	C5	N6	S7	S8	S9
HOMO	-0.11	-0.46	0.04	0.48	0.07	-0.04	0.56	-0.07	-0.51
LUMO	1.42	-0.46	-0.75	0.92	-0.63	-0.52	-0.49	0.34	0.28
HOMO ² /Σ%	1.16	10.22	0.09	12.41	0.30	0.10	19.36	0.38	19.99
LUMO ² /Σ%	42.55	2.84	7.76	12.66	6.80	4.97	4.64	2.34	1.63

As observed in Table III, The HOMO of H₃TMT molecule is mainly composed of atomic orbitals of N2, N4, S7 and S9, while the LUMO is C1, N4, C3, N6 and S7.

The frontier molecular orbital (FMO) theory developed by Kenichi Fukui in 1950's is a powerful practical model for describing chemical reactivity and reaction mechanism, which is focus on the HOMO and LUMO [20]. The energies of frontier molecular orbitals (ϵ_{HOMO} , ϵ_{LUMO}), energy band gap $\Delta\epsilon$ ($\epsilon_{\text{LUMO}} - \epsilon_{\text{HOMO}}$), electronegativity (χ), chemical potential (μ), chemical hardness (η), global softness (S), global electrophilicity index (ω) [21], [22] and additional electronic charge (ΔN_{max}) of H₃TMT and (HgCH₃)₃TMT have been calculated using (1)-(6) and listed in Table IV.

$$\chi = -1/2(\epsilon_{\text{LUMO}} + \epsilon_{\text{HOMO}}) \quad (1)$$

$$\mu = -\chi = 1/2(\epsilon_{\text{LUMO}} + \epsilon_{\text{HOMO}}) \quad (2)$$

$$\eta = 1/2(\epsilon_{\text{LUMO}} - \epsilon_{\text{HOMO}}) \quad (3)$$

$$S = 1/2\eta \quad (4)$$

$$\omega = \mu^2/2\eta \quad (5)$$

$$\Delta N_{\text{max}} = -\mu/\eta \quad (6)$$

TABLE IV: CALCULATED ϵ_{LUMO} , ϵ_{HOMO} , $\Delta\epsilon$, χ , μ , η , S , ω AND ΔN_{max} (IN A.U.) FOR H₃TMT AND (HgCH₃)₃TMT

Properties	E	ϵ_{HOMO}	ϵ_{LUMO}	$\Delta\epsilon$	χ
H ₃ TMT	-1474.97	-0.28	-0.07	-0.21	0.18
(HgCH ₃) ₃ TMT	-2053.58	-0.25	-0.05	-0.2	0.15
Properties	μ	η	S	ω	ΔN_{max}
H ₃ TMT	-0.18	0.11	0.053	0.15	1.67
(HgCH ₃) ₃ TMT	-0.15	0.1	0.05	0.11	1.50

The values of ϵ_{HOMO} can reflect the relative electron donor power, that is, the higher the value is, the weaker the attraction of the nucleus to the electron on the HOMO will be, and the larger the donor power is. The values of ϵ_{LUMO} can reflect the electron acceptability, the lower the value is, the stronger the electron acceptability is. The difference between ϵ_{HOMO} and ϵ_{LUMO} ($\Delta\epsilon$) is an important stability index for a molecule, the higher the value of $\Delta\epsilon$ is, the better stability the molecule has, and the lower chemical reactivity it has. Simulation results

reveal that global stability of molecule is related to its energy of frontier molecular orbital. As can be seen in Table IV, the HOMO energy level is higher, indicates that electron is readily transferred from the HOMO of a ligand to metal donation to form the metal complex, which provides useful guidelines for explaining its stability in environment.

C. Fukui Indices of H₃TMT Atoms

Fukui indices, which including nucleophilic Fukui indices and electrophilic Fukui indices are efficient to analyze the active site for reactions. Nucleophilic Fukui indices $f^+(r)$ is defined as $f^+(r) = q(r) - q^+(r)$, while electrophilic Fukui indices $f^-(r)$ is defined as $f^-(r) = q^-(r) - q(r)$, in which $q(r)$, $q^+(r)$ and $q^-(r)$ are charges of an atom in the neutral molecule, the positively charged molecule, and the negatively charged molecule respectively [23]. The greater the absolute value of $f^+(r)$, the easier the atom contributes electron; the greater the absolute value of $f^-(r)$, the easier the atom gains electron. Fukui indices calculated were listed in Table V.

As observed in Table V, the absolute values of nucleophilic Fukui indices of S7, S8 and S9 in H₃TMT are bigger than that of the other atoms, which indicates that S is easier to contribute electron for a coordination bond with Hg. So, all the S atoms in H₃TMT are the active sites for the reaction with CH₃HgCl. The absolute values of electrophilic Fukui indices of the atoms of N2, N4 and N6 in H₃TMT are bigger than the other atoms, therefore, N is easier to gain electron from metal donation to form a back-coordination. Thus, the atoms N in H₃TMT are considered as the second active site for the reaction. By comprehensive analysis and comparison the Fukui indices of H₃TMT, in combination with the compositions of HOMO and contribution of each atom in Table II, it can be concluded that all S and N atoms are the active sites for the reaction of H₃TMT with CH₃HgCl to form the metal complex of (HgCH₃)₃TMT. The metal-ligand interactions is strengthened and the stability is increased, which is in agreement with the studies of Cecconi [15], which surmised that there remained a secondary action between Hg and N.

TABLE V: CHARGES, NUCLEOPHILIC FUKUI INDICES AND ELECTROPHILIC FUKUI INDICES OF ATOMS OF H₃TMT MOLECULE

Item	C1	N2	C3	N4	C5	N6	S7	S8	S9
$q(r)$	0.24	-0.42	0.24	-0.42	0.24	-0.42	0.04	0.04	0.04
$q^+(r)$	0.23	-0.32	0.23	-0.37	0.23	-0.36	0.28	0.28	0.29
$q^-(r)$	-0.16	-0.23	-0.20	-0.16	-0.17	-0.20	0.01	0.02	0.06
$f^+(r)$	0.02	-0.10	0.01	-0.05	0.02	-0.05	-0.23	-0.23	-0.25
$f^-(r)$	-0.40	0.19	-0.45	0.26	-0.41	0.21	-0.03	-0.02	0.02

D. The Natural Atomic Charges

To further study the contribution to coordination bond and energy of charge distributions and charge transfer, the natural

population analysis (NPA) were performed. The natural atomic charges of some atoms in (HgCH₃)₃TMT and H₃TMT are listed in Table VI.

TABLE VI: THE NATURAL ATOMIC CHARGES OF SOME ATOMS IN (HGCH₃)₃TMT AND H₃TMT

H ₃ TMT			(HgCH ₃) ₃ TMT		
1 C	0.24	1 C	-0.20	13 C	-0.70
2 N	-0.42	2 N	-0.05	14 C	-0.69
3 C	0.24	3 C	-0.20	15 C	-0.69
4 N	-0.42	4 N	-0.05	16 H	0.17
5 C	0.24	5 C	-0.20	17 H	0.17
6 N	-0.42	6 N	-0.05	18 H	0.18
7 S	0.04	7 S	-0.03	19 H	0.17
8 S	0.04	8 S	-0.03	20 H	0.17
9 S	0.04	9 S	-0.03	21 H	0.17
10 H	0.13	10 Hg	0.45	22 H	0.17
11 H	0.13	11 Hg	0.45	23 H	0.17
12 H	0.13	12 Hg	0.45	24 H	0.18

Noted from the tabulation above, great changes appear in the atomic charges of N and S, which indicates that the charges redistributed when (HgCH₃)₃TMT was formed. The charge transferred from N atoms of H₃TMT to Hg, which can also imply the atoms N in H₃TMT are the second active site of the reaction.

The nature of the HOMO and LUMO also provides us with some insight into the reaction. For example, instead of the total electron density in a nucleophile, we should think about the localization of the HOMO orbital because electrons in this orbital are most free to participate in the reaction. The images of Fig. 2 and Fig. 3 show the distribution of HOMO and LUMO in H₃TMT and (HgCH₃)₃TMT respectively. We can get a clear impression of charge transfer. The frontier electron density is higher at the position of N2, N4, S7 and S9 in Fig. 2(a), while it is lower on C1, N4, C3, N6 and S7 in Fig. 2(b). Thus, the electrophile reacts with the former positions.

Fig. 2. The HOMO and LUMO of H₃TMT. Fig. 3. The HOMO and LOMO of (HgCH₃)₃TMT.

As observed in Fig. 2, the HOMO of H₃TMT molecule is mainly composed of atomic orbitals of N2, N4, S7 and S9. The strong overlaps between the metal 4d orbitals and S orbitals can compensate the large energy separations between the donor and metal acceptor orbitals, and thus strengthen the metal-ligand interactions

E. IR Spectroscopic Characteristics

The DFT (B3LYP) calculations are used to predict the harmonic frequencies of H₃TMT and (HgCH₃)₃TMT. To correct the vibrational anharmonicity, basis set truncation, and the neglected part of electron correlation, the calculated results were scaled down by a single factor (scaling factor) of 0.9614 [24]. The calculated values are given in Table VII and Table VIII, and the spectra are shown in S-Fig. 1 and S-Fig. 2 as supplementary material.

TABLE VII: IR FREQUENCIES OF H₃TMT (CM-1)

IR assignment	Cal.	Exp. [25]
N-H deformation	1485.6	1540-1526
C-S-C asymmetric	1261.2	1260-1240
Out of plane deformation of triazine	821.9	877-802

TABLE VIII: IR FREQUENCIES OF (HGCH₃)₃TMT (CM-1)

IR assignment	Cal.	Exp.*
N-H deformation	2949.6	2928
C-S asymmetric deformation	1440.1	1460
Out of plane deformation of triazine	1227.1	1242
CH ₃	1177.3	1188
C-N ring deformation	823.6	849
CH ₃	769.4	771

As observed from Table VII and Table VIII, the calculated results of vibrational frequencies are in good agreement with the experimental results.

F. NMR Spectroscopic Characteristics

¹³C NMR chemical shifts of H₃TMT were calculated with gauge including atomic orbitals (GIAO) approach. The calculated ¹³C-NMR is 180.09 ppm, quite close to the experimental result of Ionel (180.0 ppm) [26], Mary (172.2 ppm), and SDBS (171.60 ppm). The relative error is less than 5%. For (HgCH₃)₃TMT, the calculated ¹³C-NMR (C-S) is 185.95 ppm, the experimental result of Ionel is 180.0 ppm [26], the relative error is 3.30%.

IV. CONCLUSIONS

In this work we present the frontier molecular orbital energy, Fukui indices, the natural population analysis, global reactivity descriptors of heavy metal chelating agent of H₃TMT. By comprehensive analysis and comparison of the local reactivity descriptors of H₃TMT, in combination with the compositions of HOMO and contribution of each atom, we find that all S and N in H₃TMT are the active sites for the reaction with CH₃HgCl to form the metal complex (HgCH₃)₃TMT. The calculated ¹³C NMR chemical shifts and IR frequencies are in good agreement with the corresponding experimental results, which indicates the simulation is reasonable.

APPENDIX

Supplementary material associated with this article can be found.

Fig. 4. S The IR frequencies of H₃TMT.

Fig. 5. S the IR frequencies of (HgCH₃)₃TMT.

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REFERENCES

- [1] S. R. Jean-Philippe, J. A. Franklin, D. S. Buckley, and K. Hughes, "The effect of mercury on trees and their mycorrhizal fungi," *Environmental Pollution*, vol. 159, no. 10, pp. 2733-2739, 2011.
- [2] N. Dirilgen, "Mercury and lead: Assessing the toxic effects on growth and metal accumulation," *Ecotoxicology and Environmental Safety*, vol. 74, no. 1, pp. 48-54, 2011.
- [3] S. Gao, C. Ou-Yang, and L. Tang, "Growth and antioxidant responses in *Jatropha curcas* seedling exposed to mercury toxicity," *Journal of Hazardous Materials*, vol. 182, no. 1, pp. 591-597, 2010.
- [4] T. W. Clarkson, "The toxicology of mercury," *Critical Reviews in Clinical Laboratory Sciences*, vol. 34, no. 4, pp. 369-403, 1997.
- [5] C. Franciscato, L. Moraes-Silva, F. A. Duarte, C. S. Oliveira, R. P. Ineu, E. M. M. Flores *et al.*, "Delayed biochemical changes induced by mercury intoxication are prevented by zinc pre-exposure," *Ecotoxicology and Environmental Safety*, vol. 74, no. 3, pp. 480-486, 2011.
- [6] C. L. He, F. L. Ren, and X. B. Zhang, "A fluorescent chemical sensor for Hg (II) based on a corrole derivative in a PVC matrix," *Talanta*, vol. 70, no. 2, pp. 364-369, 2006.
- [7] D. W. Boening, "Ecological effects, transport, and fate of mercury: A general review," *Chemosphere*, vol. 40, no. 12, pp. 1335-1351, 2000.
- [8] P. Li, X. B. Feng, and G. L. Qiu, "Mercury pollution in Asia: A review of the contaminated sites," *Journal of Hazardous Materials*, vol. 168, no. 2, pp. 591-601, 2009.
- [9] S. R. Rieder, I. Brunner, M. Horvat, A. Jacobs, and B. Frey, "Accumulation of mercury and methylmercury by mushrooms and earthworms from forest soils," *Environmental Pollution*, vol. 159, no. 10, pp. 2861-2869, 2011.
- [10] P. B. Tchounwou, W. K. Ayensu, N. Ninashvili, and D. Sutton, "Review: Environmental exposure to mercury and its toxicopathologic implications for public health," *Environmental Toxicology*, vol. 18, no. 3, pp. 149-175, 2003.
- [11] K. Alizadeh, R. Parooi, P. Hashemi, B. Rezaei, and M. R. Ganjali, "A new Schiff's base ligand immobilized agarose membrane optical sensor for selective monitoring of mercury ion," *Journal of Hazardous Materials*, vol. 186, no. 2, pp. 1794-1800, 2011.

- [12] X. Chen, X. Xia, S. Wu, F. Wang, and X. Guo, "Mercury in urban soils with various types of land use in Beijing, China," *Environmental Pollution*, vol. 158, no. 1, pp. 48-54, 2010.
- [13] S. M. Ullrich, T. W. Tanton, and S. A. Abdrashitova, "Mercury in the aquatic environment: A review of factors affecting methylation," *Critical Reviews in Environmental Science and Technology*, vol. 31, no. 3, pp. 241-293, 2001.
- [14] F. J. Koschier, D. R. Brown, M. A. Friedman, J. E. Calkins, T. J. Miller, and R. F. McConnell, "Effect of dietary administration of the rubber curative trithiocyanuric acid to the rat," *Food and Chemical Toxicology*, vol. 21, no. 4, pp. 495-498, 1983.
- [15] F. Cecconi, C. A. Ghilardi, S. Midollini, and A. Orlandini, "Organomercury derivatives of the 2, 4, 6-trimercaptotriazine," *Journal of Organometallic Chemistry*, vol. 645, no. 1, pp. 101-104, 2002.
- [16] J. M. Seminario and P. Politzer, *Modern Density Functional Theory: A Tool for Chemistry*, Amsterdam, 1995, pp.105-110.
- [17] M. J. Frisch, G. W. Trucks, and H. B. Schlegel, *Gaussian 03 Revision B.03*, Pittsburgh PA, Gaussian, Inc., 2003.
- [18] M. L. Li, *Concise Handbook of Chemical Data*, Beijing: Chemical Industrial Press, 2003, pp.125-130.
- [19] J. M. Costa and J. M. Lluch, "The use of quantum mechanics calculations for the study of corrosion inhibitors," *Corrosion Science*, vol. 24, no. 11, pp. 929-933, 1984.
- [20] G. X. Wang, *Atomic Orbitals and Molecular Orbitals*, Beijing: High Educational Press, 1986, pp.102-121.
- [21] P. K. Chattaraj and S. Giri, "Stability, reactivity, and aromaticity of compounds of a multivalent superatom," *The Journal of Physical Chemistry A*, vol. 111, no. 43, pp. 11116-11121, 2007.
- [22] P. Geerlings, F. D. Proft, and W. Langenaeker, "Conceptual density functional theory," *Chemical Reviews*, vol. 103, no. 5, pp. 1793-1874, 2003.
- [23] J. Cruz, L. M. R. Martinez-Aguilera, and R. Salcedo, "Reactivity properties of derivatives of 2 - imidazoline: an ab initio DFT study," *International Journal of Quantum Chemistry*, vol. 85, no. 4-5, pp. 546-556, 2001.
- [24] C. Crak, Y. Sert, and F. Uzun, "Experimental and computational study on molecular structure and vibrational analysis of a modified biomolecule: 5-bromo-2'-deoxyuridine," *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 92, pp. 406-414, 2012.
- [25] M. F. Mahon, K. C. Molloy, M. M. Vente, and H. Ionel, "Unsymmetrically-substituted 2, 4, 6-trimercaptotriazine: Supramolecular self-assembly through C-S H-N hydrogen bonds in the crystal structures," *Inorganica Chimica Acta*, vol. 348, pp. 75-81, 2003.
- [26] H. Ionel, M. F. Mahon, K. C. Molloy, and M. M. Venter, "Synthesis and spectral characterisation of organotin (IV) 1, 3, 5-triazine-2, 4, 6-trithiolato complexes," *Journal of Organometallic Chemistry*, vol. 627, no. 1, pp. 6-12, 2001.

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