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QTAIM study of the bonding in triosmium trihydride cluster [Os₃(μ-H)₃(μ³-η²-CC₇H₃(2-CH₃)NS)(CO)₈]

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Abstract:

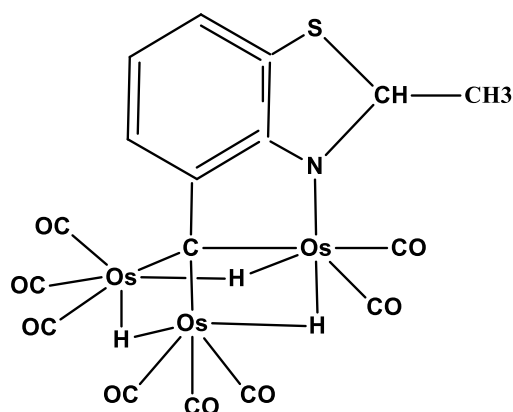
The Atoms in Molecules (AIM) analysis for triosmium cluster, which contains trihydride, carbon, carbonyl and 2-methylbenzothiazolide ligands, [Os₃(μ-H)₃(μ³-η²-CC₇H₃(2-CH₃)NS)(CO)₈] is reported. Bonding features in this cluster has been analyzed based on QTAIM ("Quantum Theory of Atoms in Molecules") in this work. The topological indices derived from electron density of relevant interactions in triosmium compound have been studied. The major interesting point of the AIM analyses is that the core of part (Os₃H₃) reveals the absence of any critical points and bond paths connecting any pairs of Os metal atoms. However, bond critical points with their bond paths occurring between all Os-H interactions were observed. For the bridged core part (Os₃H₃), a 6c–6e multicenter interaction is proposed. The topological parameters computed for the bridging 2-methylbenzothiazolide ligand interactions indicate that all of these interactions are typical related to the covalent bonds with a contribution of some double-bond character.

Keywords: DFT calculations, Osmium cluster, QTAIM bonding analysis.

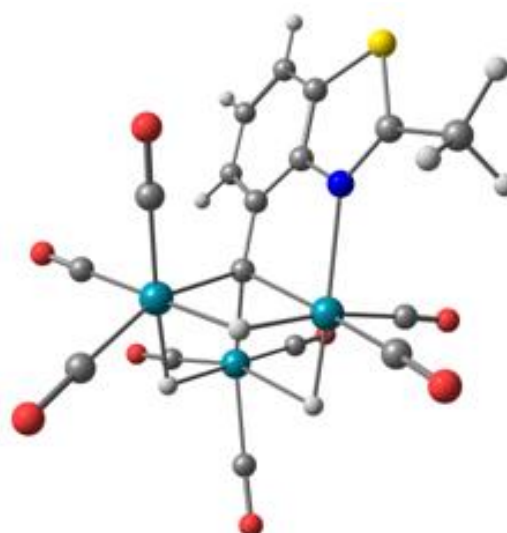
Introduction:

The reactivity of benzoheterocyclic ligands with osmium carbonyl clusters giving the electron-deficient triosmium compounds, plays a central role in organometallic chemistry. In recent years, the electron-deficient triosmium clusters have extensively been studied to model the heterogeneously catalyzed hydrodinitrification of these heterocycles (1,2). Also, these clusters have been widely used to functionalize heterocyclic substrates resulting in the synthesis of new useful compounds which are not easy to gain by using classical organic methods (3,4). The analysis of the electron density distribution, using QTAIM theory (5-9), has been considered as a good tool to analyze chemical bonds and to compare the properties of atoms and molecules (10,11). This model is very important to distinguish the existence of chemical bond interactions between any two neighbored atoms within the expression of bond critical points (BCP) along the nuclear attractors in the

neighborhood atoms (bond path, Bp), (12). Based on the QTAIM analysis, the electronic energy density $H(b)$, electron density $\rho(b)$ and Laplacian $\nabla^2\rho(b)$ calculated at critical points of the bond, offer important information about the properties of the bond. This methodology is able to a deep study of the characteristics of a metal-metal and metal-ligand interactions in cluster compounds (13). In this work, we present AIM study of triosmium cluster [Os₃(μ-H)₃(μ³-η²-CC₇H₃(2-CH₃)NS)(CO)₈] (14), shown in Fig. 1, focusing on the bonding behaviour between various atomic interactions, such as Os–Os, Os–H_{bridged}, Os–C_{bridged} and Os–C_{carbonyl} interactions. The complex under this study has been chosen due to the lack of any previous AIM study on triosmium compound contains tribridging hydride ligands and bridging C spans the Os–Os edges. In addition, this work also discusses and compares between different topological properties of a variety interactions in M–M and M–L.



(i)



(ii)

Figure 1. (i) Schematic structure and (ii) optimized geometry of triosmium cluster.

Theoretical Methods:

The optimized geometry of the triosmium cluster was obtained from the PBE1PBE level (15) using Gaussian 09 (16) program. The SDD (17) basis set augmented with a set of *f*-polarization functions (18), was used for Os atoms. whereas 6-31G (d,p) (19) basis set was used for other atoms of (H, C, N, O and S). The cluster was also characterized by analytical calculation of frequencies and has positive eigenvalues thus confirming that the optimised geometry is minima on the potential energy surface. The QTAIM analysis was calculated using the AIM2000 package (20) at the PBE1PBE/WTBS for Os atoms (21) in conjunction with the 6-31G(d,P) basis set for other atoms.

Results and Discussion:

According to QTAIM method, the structure of a compound is totally specified by the set of critical points at which the gradient of electron density $\nabla^2\rho(b)$ is zero. The existence of a bcp and bp connecting between two neighbored atoms is taken as an indicator for the chemical bonding (22). The molecular graph for triosmium compound is presented in Fig. 2. The bcps and their bps correspond to the Os-H, Os-C, Os-N, C-C, C-H, C-N, and C-S bonds were clearly found. Remarkably, the results showed the lack of any bond critical point or bond path between any two of the osmium atoms. Six rcg (ring critical point) were found for the "N(1)-C(8)- S(1)-C(6)-C(7), C(2)-C(3)-C(4)-C(5)-C(6)-C(7), Os(1)-C(1)-C(2)-C(7)-N(1), C(1)-Os(1)-H(2)-Os(3), C(1)-Os(1)-H(1)-Os(2) and C(1)-Os(3)-H(3)-Os(2) rings".

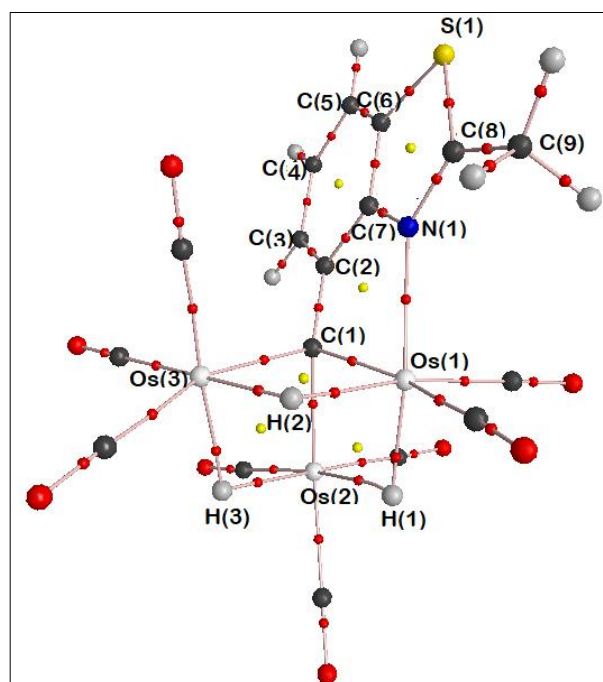


Figure 2. Molecular graph for triosmium cluster, small red balls indicate bond critical points, yellow balls indicate ring critical points and solid lines indicate bond paths.

A gradient trajectory map of (Os(1)-H(1)-Os(2)-H(3)-Os(3)-H(2)-Os(1)-C(1)) core is shown in Fig. 3. This figure shows the absence of bond critical points as well as bond paths link any pair of osmium atoms. Whereas, in the same plane, the bond paths as well as bond critical points can be observed between osmium metal atoms and bridged hydride atoms.

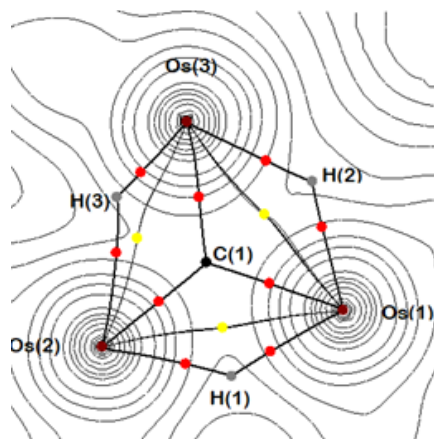


Figure 3. Gradient trajectory map of the Os(1)-H(1)-Os(2)-H(3)-Os(3)-H(2)-Os(1)-C(1) plane.

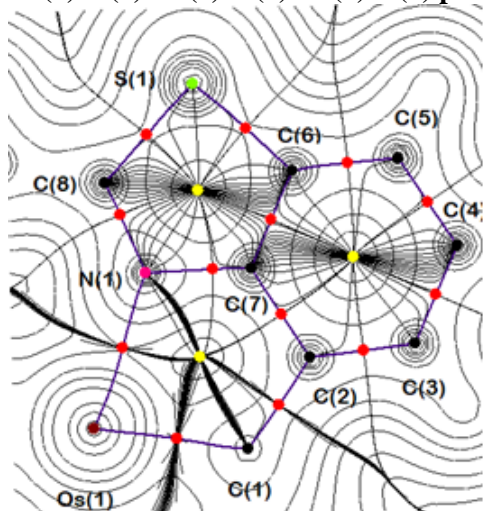


Figure 4. Gradient trajectories map of the bridging 2-methylbenzothiazolide ligand (showing bps, bcps and the atom basins).

A gradient trajectory map for 2-methylbenzothiazolide ligand, presented in Fig. 4, clearly shows the bond and ring critical points linked by bond paths associated with this ligand. For the interactions of Os(1) and C(1) with the 2-methyl benzo thiazolide, the bps and bcps can also be observed.

The Nature of the Interactions in the Core:

Within the QTAIM paradigm, at the bond critical point, calculated topological properties such as the electron density (ρ_b), Laplacian ($\nabla^2\rho_b$) and electronic energy density (H) award important insights into characteristic of the atomic interactions. The atomic interactions with the large ρ_b values (the contraction of electronic charge in the interatomic surface), and the values of $\nabla^2\rho(b) < 0$ and $H(b) < 0$ indicate the open-shell interactions (covalent and polar bonds). Whereas the atomic interactions with the small values of ρ_b (the electronic charge is depleted in the interatomic surface), and values of $\nabla^2\rho(b)$ and $H > 0$ belong to closed-shell interactions (ionic bond) (23). From the literature (24), the electronic energy density $H(b)$ is considered to be a suitable index to characterize an interaction. This term is calculated based on the equation of $H(b) = G(b) + V(b)$, where $G(b)$ and $V(b)$ are the kinetic and potential energy densities, respectively. The energy density term is computed from the equation $1/4 \nabla^2\rho(b) = 2G(b) + V(b)$. The results of topological indexes for the Os cluster are given in Table 1.

Table 1. The topological indexes calculated at bcps of the studied cluster.

"Where (ρ_b) electron density($\text{e}\text{\AA}^{-3}$), ($\nabla^2\rho_b$) Laplacian of the electron density($\text{e}\text{\AA}^{-5}$) (G_b) kinetic energy density ratio (he^{-1}), (V_b) potential energy density ratio (he^{-1}), (H_b) total energy density ratio and (ε_b) ellipticity."

Bond	$\rho_b[\text{e}\text{\AA}^{-3}]$	$\nabla^2\rho_b[\text{e}\text{\AA}^{-5}]$	$G_b[\text{he}^{-1}]$	$H_b[\text{he}^{-1}]$	$V_b[\text{he}^{-1}]$	ε_b
Os(1)-H(1)	0.109	0.165	0.086	-0.045	-0.131	0.027
Os(1)-H(2)	0.071	0.194	0.065	-0.016	-0.081	0.058
Os(2)-H(1)	0.045	0.113	0.033	-0.005	-0.038	0.619
Os(2)-H(3)	0.074	0.184	0.064	-0.018	-0.083	0.124
Os(3)-H(2)	0.085	0.188	0.072	-0.025	-0.097	0.048
Os(3)-H(3)	0.080	0.190	0.070	-0.022	-0.092	0.048
Os(1)-C(1)	0.116	0.192	0.0936	-0.046	-0.139	0.024
Os(2)-C(1)	0.131	0.230	0.113	-0.056	-0.169	0.040
Os(3)-C(1)	0.108	0.184	0.086	-0.040	-0.126	0.059
Os-C(CO)*	0.154	0.558	0.206	-0.066	-0.272	0.081
Os(1)-N(1)	0.082	0.373	0.106	-0.0130	-0.119	0.197
N(1)-C(7)	0.301	-0.806	0.210	-0.411	-0.621	0.115
N(1)-C(8)	0.356	-0.863	0.327	-0.543	-0.870	0.238
S(1)-C(6)	0.204	-0.379	0.062	-0.156	-0.218	0.190
S(1)-C(8)	0.207	-0.387	0.066	-0.162	-0.228	0.268
C(8)-C(9)	0.258	-0.629	0.068	-0.225	-0.293	0.049
C-O*	0.460	0.511	0.926	-0.798	-1.724	0.001

* Average values.

The main point of interest, as mentioned above, is the full absence of any bond critical point between Os atoms of the core which are bridged by both H and C atoms. This finding is significant since it is attributed to the absence of any trace of localized electron density between Os atoms. Therefore, it can be concluded that there are no features of chemical bonding between any pair of Os atoms in the core (22). The strong ligand bridging interaction (H and C groups) destroys the topological Os-Os. Bond critical points with their bond paths, have been observed between supported and unsupported metal-metal atoms interaction (25-26). For Os-H bonds, the topological properties were calculated as presented in Table 1. The calculated electron density values are significantly

greater than zero ($0.045 - 0.109 \text{ eÅ}^{-3}$), the Laplacian values are positive ($0.113 - 0.194 \text{ eÅ}^{-5}$) and the negative values for H(b) ($-0.005 - -0.045 \text{ eÅ}^{-1}$). According to these data and as argued in the Literature (27), Os-H interactions are classified as an open-shell model. Furthermore, the computed AIM ellipticities for Os-H bonds are greater than zero (of positive values), pointing out that these interactions are approximately a straight bonding. The plot of Laplacian map for the cluster core (Fig. 5-i) shows the polarization of the valence shell charge concentration (VSCC) of bridging hydrides toward the midpoint of Os, Os interactions. Whereas, the VSCC of the carbonyl C atoms are polarized toward the Os (3) atom (Fig. 5-ii) (28).

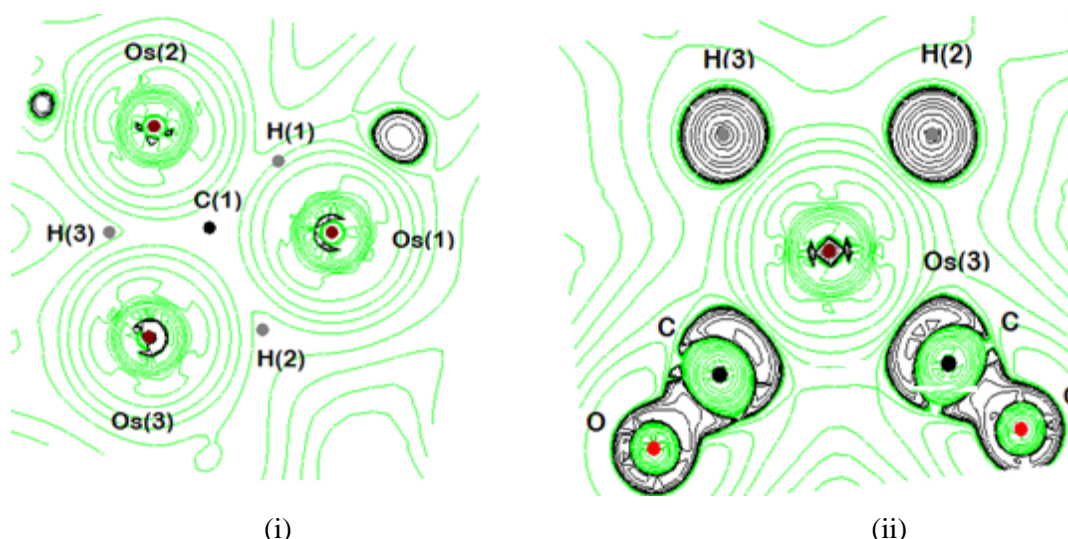


Figure 5. Laplacian distribution $\nabla^2\rho(\mathbf{r})$ plot of the triosmium cluster through (i) Os (1)-H (3)- Os (2)-C (1) plane. (ii) Os (3) with H(2) and H(3) and CO ligands plane.

As mentioned above, the absence of a bcps between any pair of the Os metal atoms limits the interpretation of the Os-Os interaction. Instead, the delocalization index, $\delta(A, B)$ (29), is a measure of the electrons shared between two atoms. This index can be considered as an appropriate AIM indicator to characterize the chemical bonding between atoms which do not depend on the existence of a bond critical point. The values of delocalization index $\delta(A-B)$ computed for Os cluster are presented in Table 2. The magnitude of $\delta(\text{Os}, \text{Os})$ is within range 0.158-0.172 and this, in fact, is very similar to that computed by Cabeza group (28) for the Os...Os interaction (within the range 0.171-0.177) in the bridged form of $[\text{Os}_3(\text{I-H})(\text{I-OH})(\text{CO})_{10}]$, and $[\text{Os}_3(\text{I-H})(\text{I-Cl})(\text{CO})_{10}]$, which possesses no direct Os...Os bond. Furthermore, the $\delta(\text{Os}, \text{Os})$ computed data are similar to, or even greater than, many other published bridged M-M compounds (13,27,30). On the other hand, those data are not comparable to

those values computed for unbridged Os-Os bonds in $[\text{Os}_3(\text{I-H})(\text{I-OH})(\text{CO})_{10}]$ and $[\text{Os}_3(\text{I-H})(\text{I-Cl})(\text{CO})_{10}]$ (28) 0.461 and 0.462, respectively. This finding leads us to conclude that the delocalization index is very useful to study ligand bridged M-M interactions. Then, by summarizing the data (summation of the delocalization indexes values of three Os...Os nonbonding and six Os-H bonding interactions), it can be concluded that the total $\delta_{(A-B)}$ for the core is 3.06 electron pairs in the core part (Os_3H_3). Therefore, the interaction in this core can be described as a 6c-6e interaction.

Table 2. Calculated delocalization indexes for triosmium cluster.

Atom pairs (A, B)	$\delta(A, B)$	Atom pairs (A, B)	$\delta(A, B)$ **
Os(1)---Os(2)	0.172	Os(3)---H(1)	0.008
Os(1)---Os(3)	0.158	Os(3)-H(2)	0.498
Os(2)---Os(3)	0.172	Os(3)-H(3)	0.395
Os(1)-H(1)	0.558	Os(1)-C(1)	0.772
Os(1)-H(2)	0.405	Os(2)-C(1)	0.804
Os(1)---H(3)	0.009	Os(3)-C(1)	0.777
Os(2)-H(1)	0.254	Os(1)-N(1)	0.422
Os(2)---H(2)	0.007	Os(2)---N(1)	0.008
Os(2)-H(3)	0.455	Os(3)---N(1)	0.009

* Average values.

** (δ_{AB}) delocalisation indices

Os-C(1), Os-C(CO) and Os-N(1) Interactions.

The computed topological values for Os-C(1) and Os-C(CO) bonds are listed in Table 1 and they show a clear variation. These bonds have obviously an open-shell bonding features, which point toward low positive values of $\nabla^2\rho(b)$ (between 0.108 to 0.116 $\text{e}\text{\AA}^{-5}$ for Os-C(1) and 0.150 to 0.158 $\text{e}\text{\AA}^{-5}$ for Os-C(CO), and a negative values for $H(b)$ (between 0.040 to 0.056 he^{-1} for Os-C(1) and -0.062 to -0.070 he^{-1} for Os-C(CO)). Rather interestingly, the Os-C(CO) have topological parameter values significantly greater than Os-C(1). Moreover, the topological values of the bridging C ligand are very similar to those calculated for bridging H and comparable to the results of bridging CO ligand of $[\text{FeCo}(\text{CO})_8]$ (31), bridging H on $[\text{Cr}_2(\mu\text{-H})(\text{CO})_{10}]$ (32) and bridging CH on $[\text{Ru}_3(\mu\text{-H})_2(\mu^3\text{-MeImCH})(\text{CO})_9]$ (13). Concerning to the calculated data of Os(1)-N(1) bond, the property of this bond is typical for the open-shell interaction with a small positive value of $\nabla^2\rho(b)$ (0.373 $\text{e}\text{\AA}^{-5}$), a low $\rho(b)$ value (0.082 $\text{e}\text{\AA}^{-3}$), and a negative of $H(b)$ value close to zero (-0.013 he^{-1}).

C-N, C-S and C-C Interactions in the 2-Methylbenzothiazolide Ligand.

The topological properties of the atom-atom interactions in bridging 2-methylbenzothiazolide ligand are presented in Tables 1. In this ligand, the nature of the bonding may also be appreciated in the graphically representations of the gradient map (shown in Fig. 4) and the Laplacian map (depicted in Fig. 6). Those two maps clearly show all the bond critical point, bond paths and atomic basins which existed in the bridging 2-methylbenzothiazolide ligand. Also, the polarization of the VSCCs of the bridging ligand C(1) is shifted toward the interatomic surface of Osmium atoms (Fig. 6), whereas the N(1) polarised to the Os(1). The topological parameters computed for the bonds

within bridging 2-methylbenzothiazolide, presented in Table 1, are typical for covalent interactions, with values for $\rho(b)$ higher than zero and a significantly negative $\nabla^2\rho(b)$ and $H(b)$ values, with some degree of delocalization (22,33-35).

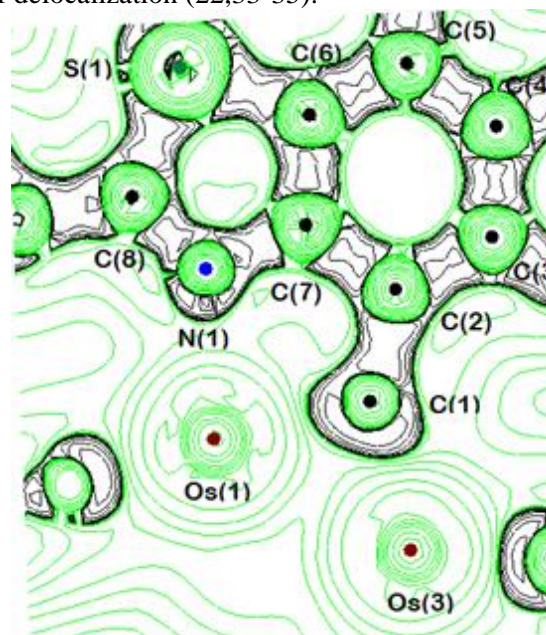


Figure 6. Laplacian distribution $\nabla^2\rho(b)$ plot of the triosmium cluster through the Os(1)-Os(2)-C(1)-N(1) plane

Regarding the N(1)-C(7) and N(1)-C(8) interactions, it is very important to compare their topological parameters with the C(6)-S(1) and C(8)-S(1) bonds. The computed electron density $\rho(b)$ and $H(b)$ for N-C bonds slightly higher than S-C bonds and this finding indicates that the former has a slightly double bond character.

Conclusion:

Topological properties of electron density for triosmium cluster $[\text{Os}_3(\mu\text{-H})_3(\mu^3\text{-}\eta^2\text{-CC}_7\text{H}_3(2\text{-CH}_3)\text{NS})(\text{CO})_8]$ have been calculated and interpreted based on AIM theory. Also, the bonding features in this cluster have been analyzed. The AIM analyses of the core part, Os_3H_3 , reveals the existence of a bond critical point and its bond path within Os-H bond. Conversely, no bond critical points linked by bond paths between any pair of Os metal atoms are observed. However, a delocalization index has been computed. The interaction in the Os_3H_3 core can be described as a multiple 6c-6e interaction. The numerical values of the topological indices of the bridging 2-methylbenzothiazolide ligand interactions indicate that all the bonds are typical for covalent bonding mode with a slight degree of double-bond character.

Authors' declaration:

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are mine ours. Besides, the Figures and images, which are not mine ours, have been given the permission for re-publication attached with the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee in University of Kufa.

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استخدام نظرية الكم للذرات في الجزيئات في دراسة الترابط الكيميائي للمركب الجسري ثلاثي هيدريد ثلاثي الاوزونيوم العنقودي $[Os_3(\mu-H)_3(\mu^3-\eta^2-CC_7H_3(2-CH_3)NS)(CO)_8]$

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الخلاصة:

تم استخدام طريقة تحليل الذرات في الجزيئات في دراسة التأثيرات في المركب العنقودي ثلاثي الاوزميوم الحاوي على اليكاندات ثلاثي هيدريد والكربون والكربونيل و 2-ميثيل بنزوئيازولايدي. تم تحليل وضع الترابط في المركب العنقودي $[Os_3(\mu-H)_3(\mu^3-\eta^2-C_7H_3(2-CH_3)NS)(CO)_8]$ باستخدام نظرية الكم للذرات في الجزيئات. تمت دراسات المؤشرات التبولوجية المستمدة من الكثافات الإلكترونية للمركب الاوزميوم العنقودي. النقطة الرئيسية المهمة في البحث هي نتائج تحليلات الذرات في الجزيء للمركز Os_3H_3 والتي دلت على غياب الروابط او النقاط الحرجة بين ذرات الاوزميوم. مع ذلك، لوحظت النقاط الحرجة مع المسارات الرابطة بين جميع الروابط بين الاوزميوم والهايديرينات $(Os-H)$. في الجزء الجسري Os_3H_3 يمكن وصف التأثير الموجود فيه بكونه من نوع سداسي المركز سداسي الالكترون $(6C-6e)$. تشير المعلومات التبولوجية المحسوبة لليكاند 2-ميثيل بنزوئيازولايدي الجسري إلى أن جميع التأثيرات فيه هي روابط تساهمية مع بعض المساهمة للروابط المزدوجة.

الكلمات المفتاحية: نظرية دالة الكثافة، الاوزميوم العنقودي، تحليل التاصر QTAIM.