A Theoretical Investigation of Chemical Bonding of a Heterometallic Trinuclear Cluster Containing Iridium and Ruthenium: [(Cp*Ir) (CpRu)₂ (μ₃-H) (μ-H)₃] by QTAIM Approach

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Abstract:
Numerous integral and local electron density’s topological parameters of significant metal-metal and metal-ligand bonding interactions in a trinuclear tetrahydrido cluster [(Cp* Ir) (CpRu)₂ (μ₃-H) (μ-H)₃] (Cp = η⁵-C₅Me₅, (Cp* = η⁵-C₅Me₄Et) were calculated and interpreted by using the quantum theory of atoms in molecules (QTAIM). The properties of bond critical points such as the delocalization indices δ (A, B), the electron density ρ(r), the local kinetic energy density G(r), the Laplacian of the electron density ∇²ρ(r), the local energy density H(r), the local potential energy density V(r) and ellipticity ε(r) are compared with data from earlier organometallic system studies. A comparison of the topological processes of different atom-atom interactions has become possible thanks to these results. In the core of the heterometallic tetrahydrido cluster, the Ru₂IrH₄ part, the calculations showed that there are no bond critical points (BCPs) or identical bond paths (BPs) between Ru-Ru and Ru-Ir. The distribution of electron densities is determined by the position of bridging hydride atoms coordinated to Ru-Ru and Ru-Ir, which significantly affects the bonds between these transition metal atoms. On the other hand, the results confirm that the cluster under study contains a 7c–11e bonding interaction delocalized over M₃H₄, as shown by the non-negligible delocalization index calculations. The small values for ρ(b) above zero, together with the small values, again above zero, for Laplacian ∇²ρ(b) and the small positive values for total energy density H(b), are shown by the Ru-H and Ir-H bonds in this cluster is typical for open-shell interactions. Also, the topological data for the bond interactions between Ir and Ru metal atoms with the C atoms of the cyclopentadienyl Cp ring ligands are similar. They show properties very identical to open-shell interactions in the QTAIM classification.

Keywords: Bonding analysis for the trinuclear cluster, DFT calculation, QTAIM approach, Topological properties, and Trinuclear tetrahydrido cluster.

Introduction:
Over the past years, several studies have been reported on the activation of transition metal clusters in inorganic and organometallic chemistry due to their possible uses in catalytic or stoichiometric reactivity. These cluster complexes, which differ from mononuclear complexes in reactivity, can coordinate with substrate molecules many times and form a multi-electron transfer to the substrate. In the polyhydrido clusters, the releasing of bridging hydrido ligands play an important spontaneously introducing multiple unoccupied coordination sites on the neighboring metal centers. Based on the very high electron density at the transition metal atoms of the polyhydrido clusters having cyclopentadienyl ligands, Suzuki et al. argued that the reactivity was increased toward the splitting of
inactive chemical bonds, such as the C−C and C−H bonds of alkanes. In terms of computational methods, Bader’s “theory of atoms in molecules (QTAIM)” simulations can be used to study the bonding and predict the properties of molecular structures. The key concept in the QTAIM theory is the distribution function of the electron density $\rho(r)$. The topological properties of $\rho(r)$ and its derivatives can play an important role in the concept of the metal-ligand and metal-metal interaction in organometallic compounds through valence bonds and non-valence interactions. Unfortunately, the topology of the electron density in trinuclear heterometallic clusters having Iridium transition metals is still not fully understood. Therefore, to offer a rather satisfying interpretation of the bonding interactions in these important classes of clusters, more QTAIM studies are needed. This work aims to study the bonding by analyzing the electron density distributions and comparing different topological indicators for Ru-Ir, Ru-Ru, Ir-H, Ru-H, Ru-C, and Ir-C bonds in trinuclear heterometallic tetrahydrido cluster: [(Cp*Ir) (CpRu)2 (μ3-H) (μ-H)3] (Cp = η5-C5Me5), (Cp* = η5-C5Me4Et), as displayed in Fig. 1. Also, the bridging hydride ligands in the trinuclear heterometallic cluster can be used as a model to study the influence of the bridging hydride atoms on the different Ru-Ru and Ru-Ir interactions. This study presents an excellent chance to investigate the topological characteristics of various bonding interactions inside this cluster.

**Computational Methods**

In this work, the DFT calculations for heterometallic tetrahydrido cluster 1 were done with the GAUSSIAN09 program and PBE1PBE functional. In this study, we used the X-ray diffraction structure for this cluster, found by Suzuki and his co-workers, as a basis for geometrical optimization. The LANL2DZ basis set was used to calculate the metal atoms Ru and Ir, while the remaining atoms were described using a 6-31G (d, p) basis set. For the QTAIM calculations, we have used the AIM2000 program package. The PBE1PBE density functional was used to perform these calculations on the theoretically optimized geometries. The large all-electron "well-tempered basis set" WTBS was used for the Ru and Ir atoms, while the 6-31G (d, P) basis set was used for the remaining atoms.

**Results and Discussion:**

**Electron Density Topological Analysis**

In the present paper, we first investigate the presence of bonding interactions in the trinuclear heterometallic tetrahydrido cluster 1 [(Cp*Ir) (CpRu)2 (μ3-H) (μ-H)3] by using the QTAIM approach.
Applying this method to cluster 1 gives the complete set of bond critical points (BCPs) together with the bond paths (BPs) that relate the bonded atoms and ring critical points (RCPs). Fig. 2 presents the molecular graph of the cluster.

Figure 2. Molecular graph of the trinuclear heterometallic tetrahydrido cluster 1, where highlights gray lines represent (BPs bond pathways), small red circles represent (BCP critical bonding points between two atoms), yellow circles represent (ring critical points RCPs) and green circles represent (critical cage CCPs).

The BCPs and their BPs for the Ir-H, Ru-H, C-H, Ir-C, Ru-C, and C-C bonds were found using the molecular graph. Remarkably, the Ru$_3$IrH$_4$ core has no BCPs and BPs between the hydride-bridge transition metal atoms, Ir, Ru (1), and Ru (2). Then, we can assume that no direct Ru-Ru and Ru-Ir bonding exists$^{25}$. Other ligands in bridging sites, such as carbonyl$^{26}$, $^{27}$, Borylenes$^{28}$, and Alkynes$^{29}$, have also shown this loss of M-M bond paths. Furthermore, RCPs located slightly closer to the geometrical centers of each Ru$_1$-$\mu_2$H$_1$-Ru$_2$-$\mu_3$H$_4$, Ru$_2$-$\mu_2$H$_2$-Ir-$\mu_3$H$_4$, Ru$_1$-$\mu_2$H$_3$-Ir-$\mu_3$H$_4$, and Cp ligands were observed for cluster 1. A significant point of interest in this cluster is no direct bond-bond interaction between the transition metal atoms because no bond critical points and bond paths are observed between the metal atoms. The absence of bond paths (BCPs) hence, has no direct bonding interaction between these Ru-Ru and Ru-Ir metallic atoms.

Figure 3. Gradient trajectories in the Ir-H(2)-Ru(2)-H(1)-Ru(1)-H(3) with H(4) plane mapped on an electron density plot, with atomic basins (BP’s) and (BCP’s).

In Fig. 3, a gradient map for core plane Ru(1)-H(1)-Ru(2)-H(3) and ($\mu_3$-H) with Ru(1), Ru(2), and Ir, all bond critical points and bond paths with the atomic basins in the chosen planes are seen. In addition, the electron density distribution is very similar. It shows a significant charge density distribution around transition metal atoms Ru and Ir but no BCPs and BPs between Ru$_1$-Ru$_2$, Ru$_1$-Ir, and Ru$_2$-Ir. The BPs and BCPs located between Ru$_1$-H, Ru$_2$-H, and Ir-H are also shown.
Figure 4. Gradient trajectories in the Cp ligand-Ir plane with atomic basins (BCP’s) and (BP’s).

Fig. 4 shows the BPs, BCPs, and RCPs associated with the CP* ligand attached to the iridium atom and electron density’s gradient map in this plane. The BCPs and BPs, found between Ir with the five carbons CP* atoms (C(11), C(12), C(13), C(14), and C(15)), located in and out of this plane, can also be observed. Additionally, H(1) and H(3) are shown on this plane.

Atoms in Molecules Analysis

The computed topological properties of the interactions between coordination bonds in the trinuclear heterometallic tetrahydrido cluster I are summarized in Table 1.

Table 1. The topological parameters at BCPs [(ρb) electron density, (∇²ρb) Laplacian, (Hb) ratio of total energy density, (Gb) ratio of kinetic energy density, (Vb) viral energy density, and (εb) ellipticity].

<table>
<thead>
<tr>
<th>Bond</th>
<th>ρb(eÅ⁻³)</th>
<th>∇²ρb(eÅ⁻⁵)</th>
<th>Gb(he⁻¹)</th>
<th>Hb(he⁻¹)</th>
<th>Vb(he⁻¹)</th>
<th>εb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ru1-H1</td>
<td>0.092</td>
<td>0.188</td>
<td>0.079</td>
<td>-0.032</td>
<td>-0.112</td>
<td>0.162</td>
</tr>
<tr>
<td>Ru1-H3</td>
<td>0.076</td>
<td>0.188</td>
<td>0.069</td>
<td>-0.022</td>
<td>-0.091</td>
<td>0.224</td>
</tr>
<tr>
<td>Ru1-H4</td>
<td>0.056</td>
<td>0.170</td>
<td>0.053</td>
<td>-0.011</td>
<td>-0.063</td>
<td>0.133</td>
</tr>
<tr>
<td>Ru2-H1</td>
<td>0.094</td>
<td>0.190</td>
<td>0.081</td>
<td>-0.033</td>
<td>-0.114</td>
<td>0.136</td>
</tr>
<tr>
<td>Ru2-H2</td>
<td>0.075</td>
<td>0.189</td>
<td>0.068</td>
<td>-0.021</td>
<td>-0.090</td>
<td>0.264</td>
</tr>
<tr>
<td>Ru2-H4</td>
<td>0.055</td>
<td>0.170</td>
<td>0.053</td>
<td>-0.010</td>
<td>-0.063</td>
<td>0.122</td>
</tr>
<tr>
<td>Ir-H2</td>
<td>0.113</td>
<td>0.188</td>
<td>0.094</td>
<td>-0.047</td>
<td>-0.141</td>
<td>0.088</td>
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<tr>
<td>Ir-H3</td>
<td>0.113</td>
<td>0.186</td>
<td>0.094</td>
<td>-0.047</td>
<td>-0.141</td>
<td>0.092</td>
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<tr>
<td>Ir-H4</td>
<td>0.090</td>
<td>0.198</td>
<td>0.080</td>
<td>-0.031</td>
<td>-0.111</td>
<td>0.049</td>
</tr>
<tr>
<td>Ru1-Cp</td>
<td>0.080</td>
<td>0.254</td>
<td>0.083</td>
<td>-0.019</td>
<td>-0.102</td>
<td>1.258</td>
</tr>
<tr>
<td>Ru2-Cp</td>
<td>0.082</td>
<td>0.252</td>
<td>0.083</td>
<td>-0.020</td>
<td>-0.104</td>
<td>2.031</td>
</tr>
<tr>
<td>Ir-Cp</td>
<td>0.078</td>
<td>0.252</td>
<td>0.081</td>
<td>-0.018</td>
<td>-0.099</td>
<td>1.561</td>
</tr>
<tr>
<td>Cp-Cp</td>
<td>0.284</td>
<td>-0.682</td>
<td>0.091</td>
<td>-0.262</td>
<td>-0.353</td>
<td>0.225</td>
</tr>
</tbody>
</table>

*Average values.

M-M Interactions in Clusters 1

Bader’s quantum theory of atoms in molecules approach is a powerful tool to provide information about atoms and the nature of chemical bonding interaction. Based on the QTAIM theory, the investigation of topological properties like “the electron density ρb,” the Laplacian of electron density ∇²ρb, and the total energy density Hb at the BCPs” are a helpful tool for the classification of chemical bonds.

From the literature, the calculated values of negative values of ∇²ρb and Hb and large values of ρb(r) are typical of shared or open-shell (covalent) interactions. Small values of ρb, positive values of ∇²ρb, and Hb are typical of closed shell (ionic or Van der Waals) interactions. The total energy density Hb(r) is defined according to Eq. 1:

\[ H_b(r) = G_b(r) + V_b(r) \]

Where Gb(r) and Vb(r) are the kinetic and potential energy densities have been identified as a more appropriate index than Laplacian to characterize an interaction. The important point for M-M (Ru-Ir and Ru-Ru) interactions is the total absence of any BCPs between any pair of transition metal atoms, which are bridged by hydride ligands. Thus, according to these results, we may say that there is no localized electron density between the Ru…Ru
or Ru…Ir interactions. According to the QTAIM model, defining and characterizing a chemical bond is associated with a found bond critical point. The topological M…M (Ru…Ir and Ru…Ru) bonds were destroyed when the metal transition atoms were spanned by μ-H and μ₂-H bridging hydride ligands (strong interaction). Depending on what was mentioned above, we conclude that there is no bond between transition metal atoms in this cluster. The absence of BCP between the metal-metal atoms has been observed, such as in bridged M…M interaction in the compounds studied by Van der Maalen et al. [Mn₃(μ-H)₃(CO)₁₂], [TC₃(μ-H)₃(CO)₁₂], [Re₃(μ-H)₃(CO)₁₂] and bridged Os…Os in clusters [Os₃(l-H)(l-Cl)(CO)₁₀] and [Os₃(l-H)(l-OH)(CO)₁₀]. However, the BCP and its BP between the metal-metal atoms have also been observed when there are strong ligand bridging interactions (μ²-S), as in the case of Mo-Mo in the complex [Mo₃ (μ²-S) (μ²-S) Cl₃(PH₃)₆]⁺ (Feliz et al.).

### M-H Interactions in Cluster 1

For Ir-H and Ru–H interactions, according to Table 1, the electron density values at the BCPs are small, >1, within the range 0.055 to 0.113 eÅ⁻³, though the Laplacian values are also small, again >1, 0.170 to 0.193 e Å⁻⁵. These results added to the negative values for Hₜ, which are in the range -0.010 to -0.047 he⁻¹, enforce us to assume that the Ru-H and Ir-H interactions are typical of the shared or open-shell (covalent) interactions in line with that of a typical open-shell bond (intermediate between ionic and covalent bonds). However, the central hydride bridge's M-H₄(μ₃) bonds exhibit observable topological properties. For instance, it is lower in electron density and higher in the Hₜ values. In addition, the values, slightly greater than zero of the ellipticity for each of the Ru-H and Ir-H bonds are typical of the straight bonding interactions between M and H atoms.

The Laplacian map computed to plane containing (Ru₂IrH₄) is very useful for analyzing the M…M and M-H interactions, as shown in Fig. 5. The pseudo-octahedral coordination of the Ru and Ir atoms in this cluster is further evident in this figure, demonstrating how their valence shell charge depletion (VSCD) is almost perfectly cubic. Also, the VSCDs of hydrido bridge ligands are directed toward the middle distance of the two transition atoms they are bonded to. The reasons for the absence of BPs and BCPs in the shape of the Laplacian distribution between Ru…Ru and Ru…Ir suggests that there are no bonding electron pairs between these transition metal atoms.

### M-Cp Interactions in Cluster 1

The five BPs were given their BCPs between Ir and C atoms of the Cp* ligand, which is a most notable aspect of the topological analysis for the Ir-C interactions in this cluster, as shown in Fig. 6. Thus, it is fair to say that there is a real chemical bonding between Ru metal and the carbon atom of Cp* ligands, not just ‘interactions’ as previously found in other M-Cp interactions. The calculated topological parameters for Ru-C and Ir-C bonds are summarized in Table 1. From these data, we argue that the Ru-C, and Ir-C bonds interactions, belong to the transit closed-shell category with positive values for ρₜ (0.078 - 0.082e Å⁻³), the ∇²ρₜ’s small and positive values in the range of (0.252 to 0.254 e Å⁻⁵) and negative, near-zero values of Hₜ (-0.018 to -0.020 he⁻¹). These numbers are consistent with the values that have previously been published in the literature. Finally, the calculated ellipticities for the M-C bonds showed that the ellipticities average...
values of Ir-Cp* interactions (1.561) are in most cases lower than the Ru-Cp bonds (1.258-2.031). The M-C bonds have a π character, according to computed large values for the ellipticities, which is compatible with past findings based on the MO theory.43.

Figure 6. Laplacian map showing the electron density in the Ir-Cp* plane.

**Delocalization Indices.**

The delocalization index, δ(A, B), is one of the best tools to estimate the number of delocalized electron pairs between two atoms43, 44. Therefore, as listed in Table 2, we calculated these indices as a tool to analyze a multicenter bonding in this cluster from one side and to describe different M…M interaction modes from another side38.

<table>
<thead>
<tr>
<th>Atom pairs (A and B)</th>
<th>δ (A, B)</th>
<th>Atom pairs (A and B)</th>
<th>δ (A, B)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ru1-H1</td>
<td>0.536</td>
<td>Ir-H4</td>
<td>0.492</td>
</tr>
<tr>
<td>Ru1-H3</td>
<td>0.435</td>
<td>Ru1-Cp*</td>
<td>0.425</td>
</tr>
<tr>
<td>Ru1-H4</td>
<td>0.319</td>
<td>Ru2-Cp*</td>
<td>0.482</td>
</tr>
<tr>
<td>Ru2-H1</td>
<td>0.549</td>
<td>Ir-Cp*</td>
<td>0.410</td>
</tr>
<tr>
<td>Ru2-H2</td>
<td>0.431</td>
<td>Ru1…Ru2</td>
<td>0.369</td>
</tr>
<tr>
<td>Ru2-H4</td>
<td>0.316</td>
<td>Ru1…Ir</td>
<td>0.334</td>
</tr>
<tr>
<td>Ir-H2</td>
<td>0.569</td>
<td>Ru2…Ir</td>
<td>0.301</td>
</tr>
<tr>
<td>Ir-H3</td>
<td>0.625</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Average values.*

The computed delocalization indices of M...M interaction values for this cluster (0.301-0.369) are higher than the reported hydride-bridged M...M nonbonding interaction values obtained in numerous other published QTAIM investigations. These studies showed that BCPs and BPs are not located in several bridged M...M nonbonding interactions giving δ(A, B) values of 0.169-0.246, 0.177, and 0.202 for “[Ru3(μ-H)2-(μ3-MeImCH)(CO)9]”45, “[Os3(μ-H)(μ-Cl)(CO)10]”38, and “[Ru3(μ-H)(μ3-κ2-Hamphox-N, N)(CO)9]”3, respectively. Alternatively, the calculated values of delocalization indices of the nonbonding M...M interaction of cluster 1 are comparable in magnitude to values found in many bridged M-M bond interactions (weak metal-metal interaction) such as Os-Os interactions of the cluster “[Os3(μ-H)2(CO)10]”38 (0.362). As a result, it is possible to say the value of the δ(A–B) for each of the M...M bonds in cluster 1 is large enough to confirm that the M...M interaction is closer to the composition of its bond (weak metal-metal interaction) than its absence38, 46. The values found for δ(M–H) in cluster
1 (0.316-0.625) are like those obtained, for instance, for Os–H (0.426-0.449) and Ru–H (0.474) bonds of the clusters mentioned above 38,45. Also, they are lower than that calculated for the complex terminal hydrido [CrH(CO)3]− (0.59) 47 and close to [(μ-H)Cr2(CO)10]− (0.38), especially the central hydride bridge δ (M-H4) values. In summary, δ(M–H) calculations suggest that each of the four M–H bonds in cluster 1 has just half a shared pair electron. Based on the sum of the δ(A–B) for the interactions in the core part Ru2Ir(μ-H)(μ3-H) of cluster 1 (5.276), thus a multicenter 7c–11e interaction in this part of the molecule is suggested to explain the bonding in this cluster.

Conclusions:
In this study, QTAIM method was used to investigate the bonding in the trinuclear heterometallic tetrahydrido cluster [(Cp*Ir)2 Ru2 (μ3-H)2]I. The metal-ligand and metal-metal bond critical points parameters ρ(r), ∇ρ(r), G(r), H(r), V(r), and δ(A, B), as well as ellipticity, are correlated with the computed data in the former organometallic systems studies. These results allowed an excellent comparison of the topological properties of various atom-atom interactions. Our calculations suggest that a multicentre 7c–11e type exists in the bridged core part, Ru2Ir(μ3-H) (μ-H)3. Most intriguingly, the presence of bridging hydride ligands affects the electron density distribution of Ru...Ru and Ru...Ir interactions, for which no direct bonding has been observed due to the absence of BCPs and their BPs between these transition metals. The calculated topological properties of the Ru-H, Ir-H, Ru-Cp, and Ir-Cp bonds indicate that they are all typical open-shell bonds.

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Authors’ declaration:
- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are ours. Besides, the Figures and images, which are not ours, have been given the permission for re-publication attached with the manuscript.
- The author has signed an animal welfare statement.

- Ethical Clearance: The project was approved by the local ethical committee in University of Kufa.

Authors' contributions statement:
Manuscript preparation, computational analysis, and final editing were conducted by A.H. While manuscript review was made by M.A. All authors read and agreed to the published version of the manuscript.

References:


تحقيق نظري للارتباط الكيميائي لعنقود ثلاثي النوى غير متجانس يحتوي على الإيريديوم والروثينيوم: 

$\text{[(Cp}^* \text{Ir)} (\text{Cp Ru})_2 (\mu_3\text{-H}) (\mu\text{-H})_3]\}$

الخلاصة:

تم حساب وتفسير العديد من المعلمات الطبولوجية المواقعية والمتكاملة لكثافة الإلكترون لتفاعلات ترابط المعادن مع المعادن والروابط المعدنية المهمة في المركب العنقودي رباعي النوى رباعي هيدريدود 

$\text{[(Cp}^* \text{Ir)} (\text{Cp Ru})_2 (\mu_3\text{-H}) (\mu\text{-H})_3]\} I (\text{Cp} = \eta^5\text{-C}_{5}\text{Me}_5), (\text{Cp}^* = \eta^5\text{-C}_{5}\text{Me}_4\text{Et})$

تم حساب وتفسيرها باستخدام نظرية الكم للذرات في الجزيئات (QTAIM). تم مقارنة خصائص النقاط الحرجة للأواصر مثل مؤشرات اللوكات للكثافة الكبيرة للكثافة $\rho(r)$، وكثافة الطاقة الحركية الموقعة $V(r)$، وكثافة الطاقة الكامنة الموقعة $H(r)$، وكثافة الطاقة الكامنة الموقعة $V(r)$، وكثافة الطاقة الكامنة الموقعة $H(r)$، وكثافة الطاقة الكامنة الموقعة $V(r)$ لقبضة الالنتبال (ذرة مع ذرة) المختلفة. تُظهر التفاعلات التي تم حسابها في المركب العنقودي للتفاعلات بين ذرات هيدريدود، وهذا له تأثير كبير على تكوين الأواصر بين ذرات المعادن الانتقالي. من ناحية أخرى، تؤكد النتائج أن الكتلة قيد الدراسة تحتوي على تفاعلات ترابط $7c-11e$ غير محدد على $\text{M}_2\text{HS}_3$, كما هو موضح في حسابات مؤشر التفاعلات التي تم حسابها في المركب العنقودي للتفاعلات بين ذرات هيدريدود. وتظهر القم الصغرى للكثافة $\rho(b)$ فوق الصفر، جنبًا إلى جنب مع الفجوة الصغرى في النقطة القطبية $\text{Laplacian}$ $\nabla^2 \rho(b)$ على $\text{Ir-H}$ و $\text{Ir-Ru}$ في هذا المركب العنقودي نموذجًا لتفاعلات الغلاف المفتوح أيضًا، وتتشابه الفترات الطيفية لتفاعلات الروابط بين ذرات المعادن $\text{Ru}$ و $\text{Ir}$ مع ذرات $\text{C}$ من بروابط حلقة $\text{cyclopentadienyl Cp}$، وظهور توزيعات الإهليلجية $\text{H}(b)$، بواسطة روابط $\text{Ru-H}$ و $\text{Ir-H}$ في هذا المركب العنقودي نموذجًا لتفاعلات الغلاف المفتوح أيضًا، وتتشابه الفترات الطيفية لتفاعلات الروابط بين ذرات المعادن $\text{Ru}$ و $\text{Ir}$ مع ذرات $\text{C}$ من بروابط حلقة $\text{cyclopentadienyl Cp}$، وظهور توزيعات الإهليلجية $\text{H}(b)$، بواسطة روابط $\text{Ru-H}$ و $\text{Ir-H}$ في هذا المركب العنقودي نموذجًا لتفاعلات الغلاف المفتوح أيضًا، وتتشابه الفترات الطيفية لتفاعلات الروابط بين ذرات المعادن $\text{Ru}$ و $\text{Ir}$ مع ذرات $\text{C}$ من بروابط حلقة $\text{cyclopentadienyl Cp}$، وظهور توزيعات الإهليلجية $\text{H}(b)$، بواسطة روابط $\text{Ru-H}$ و $\text{Ir-H}$ في هذا المركب العنقودي نموذجًا لتفاعلات الغلاف المفتوح أيضًا، وتتشابه الفترات الطيفية لتفاعلات الروابط بين ذرات المعادن $\text{Ru}$ و $\text{Ir}$ مع ذرات $\text{C}$ من بروابط حلقة $\text{cyclopentadienyl Cp}$، وظهور توزيعات الإهليلجية $\text{H}(b)$، بواسطة روابط $\text{Ru-H}$ و $\text{Ir-H}$ في هذا المركب العنقودي نموذجًا لتفاعلات الغلاف المفتوح أيضًا، وتتشابه الفترات الطيفية لتفاعلات الروابط بين ذرات المعادن $\text{Ru}$ و $\text{Ir}$ مع ذرات $\text{C}$ من بروابط حلقة $\text{cyclopentadienyl Cp}$، وظهور توزيعات الإهليلجية $\text{H}(b)$، بواسطة روابط $\text{Ru-H}$ و $\text{Ir-H}$ في هذا المركب العنقودي نموذجًا لتفاعلات الغلاف المفتوح أيضًا، وتتشابه الفترات الطيفية لتفاعلات الروابط بين ذرات المعادن $\text{Ru}$ و $\text{Ir}$ مع ذرات $\text{C}$ من بروابط حلقة $\text{cyclopentadienyl Cp}$، وظهور توزيعات الإهليلجية $\text{H}(b)$، بواسطة روابط $\text{Ru-H}$ و $\text{Ir-H}$ في هذا المركب العنقودي نموذجًا لتفاعلات الغلاف المفتوح أيضًا، وتتشابه الفترات الطيفية لتفاعلات الروابط بين ذرات المعادن $\text{Ru}$ و $\text{Ir}$ مع ذرات $\text{C}$ من بروابط حلقة $\text{cyclopentadienyl Cp}$، وظهور توزيعات الإهليلجية $\text{H}(b)$، بواسطة روابط $\text{Ru-H}$ و $\text{Ir-H}$ في هذا المركب العنقودي نموذجًا لتفاعلات الغلاف المفتوح أيضًا، وتتشابه الفترات الطيفية لتفاعلات الروابط بين ذرات المعادن $\text{Ru}$ و $\text{Ir}$ مع ذرات $\text{C}$ من بروابط حلقة $\text{cyclopentadienyl Cp}$، وظهور توزيعات الإهليلجية $\text{H}(b)$، بواسطة روابط $\text{Ru-H}$ و $\text{Ir-H}$ في هذا المركب العنقودي نموذجًا لتفاعلات الغلاف المفتوح أيضًا، وتتشابه الفترات الطيفية L

الكلمات المفتاحية: تحليل الترابط للكتلة ثلاثية النوى، وحساب DFT، طريقة JTAIM، والخصائص الطيفية، والكتلة ثلاثية النوى.