The QTAIM Approach to Chemical Bonding in Triruthenium Carbonyl Cluster: \([\text{Ru}_3 (\mu - \text{H})(\mu_3-\kappa^2-\text{Haminox-N,N})(\text{CO})_9]\)

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Abstract. The bonding in the hydride triruthenium carbonyl cluster \([\text{Ru}_3 (\mu - \text{H})(\mu_3-\kappa^2-\text{Haminox-N,N})(\text{CO})_9]\) is investigated by using the Quantum Theory of Atoms-in-Molecules (QTAIM). Calculated metal–metal and metal–ligand bond critical points (bcp) properties, electron density \(\rho(b)\), Laplacian \(\nabla^2 \rho(b)\), local energy density \(H(b)\), local kinetic (Lagrangian) energy density \(G(b)\), local potential energy density \(V(b)\) ellipticity \(\ell(b)\), and bond delocalization indices \(\delta(A, B)\) are consistent with the relevant transition metal clusters in the literature. The topological data recognizes bond paths (bp) and bond critical points for metal–metal interactions in the core of the hydride triruthenium cluster \([\text{Ru}(1)-\text{Ru}(3)\text{ and Ru}(2)-\text{Ru}(3)]\). However, no direct bond path is found for the interaction between the hydride bridged Ru atoms, while a non-negligible delocalization index \(\delta(\text{Ru}(1)\text{...Ru}(2))\) is obtained for this non-bonding interaction. An interaction of 5-center 6-electron type is proposed for the core. The topological parameters of Ru-N oxazoline ring bond suggest a pure \(\sigma\)-bond.

1. Introduction.

The interest in synthetic chemistry is focused on the preparation of novel chiral metal catalysts for asymmetric processes [1]. For example of chiral triruthenium clusters reported so far correspond to species containing mono- or bidentate chiral phosphane ligands. These latter complexes have been used as catalyst precursors in asymmetric isomerization, hydroformylation or hydrogenation of unsaturated substrates. In most catalytic reactions, the catalyst precursors have been prepared in situ and their nature remains unknown. No other cluster complexes containing chiral N-donor ligands have been reported to date. During the last decade, reported by Cabeza and his co-workers has thoroughly studied the synthesis and reactivity of carbonyl clusters derived from 2-aminopyridines[2]. In this paper we study one of these catalyst by QTAIM theory The important development in topological system and its ability to identify a bond between any two atoms in terms of bond paths (bps) and bond critical points (bcps)[3].

On the basis of QTAIM, the relation between bonding modes and topological properties of the electron density and its Laplacian cannot be straightforwardly extended to organometallic compounds, because of the nature of the bonding interactions between transition-metal atoms are not completely understood yet and much argue is still occurring on its actual presence, role and mechanism and the bonds in the transition metal display a different and much narrower spectrum of topological indexes. [4][5][6][7][2].

At now, a many papers have been published to study the topology of the electron density in cluster compounds that have a three or multitransition metal–metal interactions between their atoms[8][9][10][11][12][13][14][15][16][17][18][19][20]. So, more QTAIM studies applied on this class of complexes in order to discribe the relationship between metal–metal bonds and the topology of their associated electron density[21].

In this study the QTAIM topological analysis of the electron density employed in the N-Heterocyclic, mono hydride tri ruthenium clusters \([\text{Ru}_3 (\mu - \text{H})(\mu_3-\kappa^2-\text{Haminox-N,N})(\text{CO})_9]\) (Fig. 1), which was previously reported by Cabeza and his co-workers[22]. The amido fragment spans an edge...
above the metal triangle, while the N atom of the oxazoline ring is attached to the remaining metal atom. In addition, the bridging NH and H ligand spans on the Ru(1)-Ru(2), this allowing interesting comparisons between the topological properties of related but different atom-atom bonding interactions within the same molecule.

![Figure 1: geometry optimization structure of [Ru₃(μ-H)(μ₃-κ²-Hamphox-N,N)(CO)₉].](image)

2. Computational Methods
The X-ray diffraction structures of this compound was used as starting points for geometry optimization, which were performed with the GAUSSIAN03[23] and GAUSSIAN09[24] packages at the DFT level of theory, using PBE1PBE functional. 6-31G (d, p) basis set were employed for H, C, N and O atoms. The LANL2DZ effective core potential (ECP) basis set was used for Ru atoms. These calculations included both local and integral properties and were carried out with the AIM2000 programs[25]. The accuracy of the integrated properties was finally set at least at 1.0 x 10⁻⁴ (from the Laplacian of the integrated electron density), whereas the accuracy of the local properties was 1.0 x 10⁻¹⁰ (from the gradient of the electron density at the bond critical points). The AIM results described in this work corresponding to calculations performed with the PBE1PBE/WTBS/6-31G (d, P)[26][27].

3. Results and Discussion.
3.1. Topological Properties of the Electron Density
The main feature of atoms in molecules (AIM) theory of Bader[28], with the AIM2000 program package, is that the topology of electron density ρ(r) contains information about the bonding situation. Specifically, at the critical points (the points in space at which the gradient of the density vanishes [∇ρ(r) = 0]), carries important information about the multiplicity and the covalence of the bond. The critical point characterized by two negative curvatures (maximum) and one positive curvature (minimum), labelled as (3,-1), is referred to as a bond critical point (bcp) and is considered to be indicative of the presence of chemical bond, in contrast, a ring critical point (rcp) has one negative curvature and two positive curvatures, labelled as (3,+1). Some structures necessarily contain other critical point of the density: the (3,+3) is produced inside cages (cage critical point, ccp). A chemical bond between two atoms is characterized by a line of maximum electron density (the bond path, bp) which links the two atomic nuclei and intersects an interatomic surface at the bond critical point. The
chemical structure according to these descriptions is simply the topological graph produced by the maxima of the electron density and the bond paths. The image shown in (Fig. 2) was obtained by applying the QTAIM approach to this compound, it's easily observe bond and ring critical points, together with the bond paths that connect the bonded atoms through their corresponding bond critical points. The bcps and bps for the Ru-N, Ru-C, Ru-H, Ru-Ru, N-H, C-O, C-N, C-C, and C-H bonds were clearly found. Importantly, the bcp and bp related to Ru(1) and Ru(3) or between Ru(3) and Ru(2) bonds were found science no bcps or bps were observed between Ru(1) and Ru(2). Six rcps were clearly observed, corresponding to the C(4)-C(5)-C(6)-C(7)-C(8)-C(9), C(2)-C(3)-C(4)-C(9)-C(10), O(1)-C(1)-N(2)-C(3)-C(2), Ru(3)-N(2)-C(1)-N(1)-Ru(2), Ru(3)-Ru(1)-[N(1) or H(1)]-Ru(2), and Ru(1)-N(1)-Ru(2)-H(1) rings.

Figure 2: Molecular graph of the triruthenium cluster, showing the bond paths (gray lines) with the bond critical points (small red circles between two atoms) and ring (yellow circles) critical points.

A gradient trajectory map of the total electron density in the Ru(1)-Ru(2)-Ru(3) plane which described in (Fig. 3), showing the bcp and bp between Ru(1)-Ru(3) and Ru(3)-Ru(2) together with the atomic basins for these and other atoms located in the same plane. Three CO ligands, located nearly in the same plane, are also visible in the plot. The bp’s and bcps found between H(1) and Ru(1) and Ru(2) metal atoms from the other side, the bps and bcps found between N(1) and Ru(1) and Ru(2) metal atoms also located in these plane can be observed.
Figure 3: Gradient trajectories mapped on a total electron density plot in the Ru(1)-Ru(2)-Ru(3) plane, showing the atomic basins, bps and bcps.

(Fig. 4) describe a gradient trajectory map of the total electron density in the Ru(1)-H(1)-Ru(2)-N(1) plane. The bps and bcps found between the ligand [H(1) or N(2)] and Ru(2) and Ru(3) metal atoms located in these plane can also be observed.

Figure 4: Gradient trajectories mapped on a total electron density plot in the Ru(1)-H(1)-Ru(2)-N(1) plane, showing the atom basins, bps, bcps and rcp.

(Fig. 5) displays a gradient trajectory map of the total electron density in the plane spanned by the (+)-2-amino(4R,5S)-indanyl-2-oxazoline (Haminox) ligand. It shows the bps and bcps of the interactions of Ru(3) with the amino oxazoline ligand N(2) atom. On the other hand, both bps and bcps in a ring made between Ru(3)-N(2)-C(1)-N(1)-Ru(1 or 2).
3.2. Atoms in Molecules Analysis

In the framework of QTAIM, we have calculated the topological properties of the triruthenium cluster complex (Table 1).

Table 1. Selected topological properties at the critical points for triruthenium cluster.

| Bond           | ρ(b)(eÅ⁻³) | \( \nabla^2 \rho(b)(eÅ^{-5}) \) | \( G_b(he^{-1}) \) | \( H_b(he^{-1}) \) | \( V(he^{-1}) \) | \( \epsilon_b \) |
|----------------|------------|-------------------------------|-------------------|-------------------|----------------|------------|
| Ru(1)-Ru(3)   | 0.4430     | 0.6748                        | 0.2499            | -0.0812           | 0.3311         | 0.0539     |
| Ru(2)-Ru(3)   | 0.4370     | 0.6910                        | 0.2517            | -0.0790           | 0.3307         | 0.0576     |
| Ru(1,2)-N(1)(ave) | 0.7869   | -0.0929                       | 1.0250            | -0.0961           | 1.1211         | 0.0185     |
| Ru(1,2)-H(1)(ave) | 0.7665   | -0.0450                       | 0.6729            | -0.2225           | 0.8954         | 0.0723     |
| Ru(3)-N(2)    | 0.7781     | 3.8768                        | 1.0460            | -0.0768           | 1.1229         | 0.0727     |
| C(1)-N(1)     | 3.3848     | -12.6587                      | 1.8135            | -4.9781           | 6.7916         | 0.1421     |
| C(1)-N(2)     | 3.8528     | -9.9338                       | 4.2871            | -6.7705           | 11.0576        | 0.3281     |
| C(3)-N(2)     | 2.6500     | -7.4056                       | 1.2541            | -3.1055           | 4.3597         | 0.0280     |
| N(1)-H(2)     | 3.4125     | -18.0341                      | 0.5481            | -5.0566           | 5.6046         | 0.0220     |
| C(1)-O(1)     | 3.1256     | 0.0860                        | 4.1271            | -4.9873           | 9.1144         | 0.0394     |
| C(2)-O(1)     | 2.3873     | 0.0931                        | 2.3727            | -3.3036           | 5.6763         | 0.0239     |
| C(2)-C(3)     | 2.4442     | -5.5945                       | 0.5525            | -1.9511           | 2.5035         | 0.0463     |
| Ru-CO(ave)    | 1.4142     | -0.1289                       | 1.8762            | -0.5868           | 2.4630         | 0.0357     |
| C-O(ave)*     | 4.5687     | 0.1439                        | 10.5306           | -7.4839           | 18.0145        | 0.0054     |

* Average values. a Bond path length. b Electron density at the bcp. c Laplacian of the electron density at the bcp. d Kinetic energy density ratio at the bcp. e Total energy density ratio at the bcp. f Potential energy density ratio at the bcp. g Ellipticity at the bcp.

3.2.1. Ru- Ru Interactions. In the core the hydride-bridged Ru(1)-Ru(2) interaction exist no bcp's or direct bps. the values of ρ(b) for the Ru(1)-Ru(3) and Ru(2)-Ru(3) interactions are [0.4430 and 0.4370 e Å⁻³], respectively. also it have a small positive values for \( \nabla^2 \rho(b) \) [0.6748 eÅ⁻⁵ for Ru(1)-Ru(3) and 0.6910 eÅ⁻⁵ for Ru(2)-Ru(3)]. The positive value of G(b) were obtained for the both Ru(1)-Ru(3)
[0.2499 he$^{-1}$] and Ru(2)-Ru(3) [0.2517 he$^{-1}$]. Above findings suggested that the interactions between Ru(1)-Ru(3) and Ru(2)-Ru(3) are best described as typical open-shell metal-metal interactions.

The small values of $\varepsilon_b$ [0.0539 and 0.0576] are comparable to those reported for Os-Os bonds in [Os$_2$(CO)$_{12}$], [Os$_2$(H)(μ-Cl)(CO)$_{10}$], [Os$_2$(μ-H)(μ-OH)(CO)$_{10}$], [Os$_2$(μ-H)$_2$(CO)$_{10}$][29], and Ru-Ru bonds in [Ru$_6$(CO)$_{12}$][13], and [Ru$_3$(μ-H)$_2$(μ$_3$-MeImCH)(CO)$_{10}$][21]. For instance, for [Os$_2$(CO)$_{12}$], the electron density $\rho$, Laplacian $\nabla^2\rho$, kinetic energy $G_b$ and ellipticity $\varepsilon_b$ values for unabridged Os-Os bond are 0.327 eÅ$^{-3}$, 0.829 eÅ$^{-3}$, 0.435 he$^{-1}$ and 0.120, respectively. The average value of the electron density of [0.7665 eÅ$^{-3}$ and 0.7869 eÅ$^{-3}$] and Laplacian of [-0.0450 eÅ$^{-3}$ and -0.0929 eÅ$^{-3}$] for Ru(1,2)-H(1) and Ru(1,2)-N(1) interactions indicated that the strength of these bonds is comparable to that of pure covalent single bonds between non-metal atoms[15][8]. Additionally, the ellipticity is [0.0723 and 0.0185], and this is comparable with [Ru$_6$(μ-H)$_2$(μ$_3$-MeImCH)(CO)$_{10}$] system (0.086)[21].

The Ru$_6$(H,N) part of the cluster can be analysed by looking at the Laplacian of the electron density at the Ru(1)-H(1) or N(1)-Ru(2)-Ru(3) plane of the molecule (Fig. 6). Valence shell charge concentration (VSCC) of bridging H(1) and N(1) atoms are polarized toward the midpoint of the Ru(1)-Ru(2) edge. A small polarisation was found, and positive values were obtained for Laplacian of Ru(1,2)-H(1) and Ru(1,2)-N(1) bcp's, (Table 1), than those expected in the absence of such polarization. One maximum of Laplacian was found for the hydrogen bridging two ruthenium atoms[21].

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{laplacian_map.png}
\caption{Laplacian map of the electron density in the Ru(1)...Ru(2)-Ru(3) plane of triruthenium cluster.}
\end{figure}

3.2.2. Delocalization Indices. The delocalization indices for the two unabridged Ru-Ru bonds. For the Ru(1)-Ru(3) and Ru(2)-Ru(3) bonds, calculated values are smaller than 0.474. This is in agreement with the few cases reported in the literature, the Ru-Ru bond showed an average value of 0.458 in [Ru$_6$(μ-H)$_2$(μ$_3$-MeImCH)(CO)$_{10}$][21], the delocalization indices of Os-Os bonds in the range of 0.350 - 0.461 for [Os$_2$(CO)$_{12}$], [Os$_2$(μ-H)(μ-Cl)(CO)$_{10}$], [Os$_2$(μ-H)(μ-OH)(CO)$_{10}$] and [Os$_2$(μ-H)$_2$(CO)$_{10}$][29] and the Fe-Fe bond indicated an average value of 0.398 in [Fe$_3$(μ-H)(μ-COMe)(CO)$_{10}$][30]. Also, similar values were observed for the indexes for other metal-metal interactions[31]. In contrast, Ru(1)...Ru(2) nonbonding interactions of this compound showed a small value for their delocalization indices (0.2007). This is comparable with the reported hydride-bridged M...M nonbonding interactions. For instance, between 0.169 and 0.246 for Ru...Ru interactions of [Ru$_6$(μ-H)$_2$(μ$_3$-
The Sixth Scientific Conference “Renewable Energy and its Applications”
IOP Conf. Series: Journal of Physics: Conf. Series 1032 (2018) 012068
doi:10.1088/1742-6596/1032/1/012068

MeImCH)(CO)₉][21], 0.177 for Os...Os interaction of [Os₃(μ-H)(μ-Cl)(CO)₁₀][29], and 0.208 for Fe...Fe interaction of Fe₃(μ-H)(μ-COMe)(CO)₁₀][2] and in line with other values found for ligand-bridged M...M interactions in several organometallic compounds[32][8]. On the other hand, the delocalization indices of the nonbonding Ru(1)...Ru(2) interaction is comparable with the previously reported for unbridged metal-metal interaction such as Co-Co interaction of [Co₃(CO)₉] (0.460)[10]. As the bridged Ru...Ru interaction of this cluster show a smaller delocalization index than that of unbridged Ru-Ru interaction.

Table 2. The delocalization indices for specific atomic δ(A, B) interactions.

| atom pairs (A, B) | δ(A, B) | atom pairs (A, B) | δ(A, B) |
|------------------|---------|------------------|---------|
| Ru(1)-Ru(3)      | 0.5028  | C(2)-O(1)        | 0.7790  |
| Ru(2)-Ru(3)      | 0.4849  | O(1)-C(1)        | 0.7800  |
| Ru(1,2)-H(1)     | 0.4550  | C(2)-C(3)        | 0.8070  |
| Ru(1,2)-N(1)     | 0.5080  | N(2)-C(3)        | 0.8430  |
| Ru(3)-N(2)       | 0.5079  | Ru(1)...Ru(2)    | 0.2007  |
| N(1)-C(1)        | 0.8380  | Ru(3)...N(1)     | 0.0410  |
| N(1)-H(2)        | 0.7380  | Ru(2,3)...C(1)   | 0.0210  |
| N(2)-C(2)        | 0.0110  | Ru(3)...C(3)     | 0.0150  |
|                  |         | Ru...O_{CO}      | 0.1907  |

The delocalization index of the δ(Ru-H) interactions of cluster (Table 2) has an average value of 0.455, which is almost equal to the average value of δ(Ru-H) interactions of [Ru₃(μ-H)₂(μ³-MeImCH)(CO)₉] system (0.474) [21]. Also, this is in line with few cases reported to date for the M-H interactions[31]. Interestingly, the calculated delocalization index values for the Ru(1)-H(1) and Ru(2)-H(1) suggested that a half an electron pair is shared between two Ru-H bonds. Additionally, delocalization index values of the Ru-H bonds are very similar to that of the values computed for Ru(1)-Ru(3) and Ru(2)-Ru(3) bonds, although the topology of both kinds of bonds is quite different as reflected by their local topological parameters presented in (Table 1).

It is interesting to note that the sum of all of the delocalization indices values for the bonding and non-bonding interactions in the Ru(1)-H(1),N(1)-Ru(2)-Ru(3) plane is roughly 3 electron pairs. It can be conclude that the interaction in the core part for this compound exists a five centers six electrons (5c-6e).

3.2.3. Ru-CO Interactions. The mean value of the Ru-CO interactions is presented in (Table 1). This value give an agreement with the literature[31]. The ρ_{ij} value of this bond is closed to 1.4142 Åe⁻³, which is higher than metal-metal bonds, but lower than the pure covalent single bonds between nonmetal atoms.

The value of δ(M...O_{CO}) is an indicator of the presence or absence of π-back-bonding in M-CO bonds, because the π-back-donation involves significant M...O_{CO} interactions[8]. Hence, the delocalization indices for the δ(M...O_{CO}) interactions were calculated (Table 2) to check the π-bonding in the Ru-CO unit. The average values of δ(Ru...O_{CO}) is 0.1907, and this is within the range of δ(M...O_{CO}) for Ru, Os, Co, Fe, and Ni carbonyl complexes (0.15 - 0.25)[29][21][8]. On the other hand, no π-back-donation was observed [Cu(CO)₂⁺]⁺ [δ(Cu...O_{CO}) = 0.09 for and δ(B...O_{CO}) = 0.04 for
H$_3$BCO][8]. These results are also confirmed by the topological indices of the C-O bonds calculated in (Table 1), which are consistent with a weak C-O bond compared to a H$_3$BCO.

3.2.4. Ru-N(1)oxazoline ring and Ru-N(2) Interactions. The values of the topological indices for the Ru(3) atom and N(2) atom of oxazoline ring, $\rho_b$(eÅ$^{-3}$) = 0.7781, $\nabla^2\rho_b$(eÅ$^{-5}$) = 3.8768, $G_b$(he$^{-1}$) = 1.0460, $H_b$(he$^{-1}$) = -0.0768, $V$ =1.1229, $\varepsilon_b$ = 0.0727 (Table 1). These values are similar to the bond between Ru(1) and Ru(2) with N(1) atoms [$\rho_b$(eÅ$^{-3}$) = 0.7869, $\nabla^2\rho_b$(eÅ$^{-5}$) = -0.0929, $G_b$(he$^{-1}$) = 1.0250, $H_b$(he$^{-1}$) = -0.0961, $V$ = 1.1211, $\varepsilon_b$ = 0.0185)]. Importantly, the ellipticity ($\varepsilon_b$) are (0.0727 and 0.0185) for the former and latter Ru-N bonds, these results indicate that the Ru(3)-N(2) bond has a slightly greater double bond character. The delocalization indexes computed for the two Ru-N bonds interactions are very similar, 0.510 for Ru(1)-N(1) and 0.507 for Ru(2)-N(2) and Ru(3)-N(2). These numbers indicate that about 0.5 electron pair is shared between bonded atoms. The valence shell charge concentrations (VSCCs) of both these two nitrogen atoms, as shown in (Fig. 7), are distorted toward their bonded ruthenium atoms.

![Figure 7: The Laplacian of the electron density in the Ru(1)-N(1), Ru(3)-N(2) and Ru(2)-N(2) atoms.](image)

As discussed above, the value of $\delta$(M...O$_{CO}$) is a reasonable sign of $\pi$-bonding in M-CO bonds. To establish the presence or absence of $\pi$-bonding in the Ru(1)-N(1), Ru(2)-N(1) and Ru(3)-N(2) bonds, the delocalization indices for the Ru(1)...C(1,3) and Ru(2,3)...C(1) interactions were calculated (Table 2). These values are very small and nearly equal to the delocalization indices of the Ru(3)...N(1) interactions, where no $\pi$-bonding exist. Therefore, the oxazoline ligand bonded to Ru atom behaves as a pure $\sigma$-donor.

3.2.5. C-C, C-N and C-O Interactions within oxazoline ring. The gradient trajectory maps as show in (Fig. 8) describe the bcp's and bps between the atoms of the oxazoline ligand and their atomic basins. The positions of bcp's are not symmetrical, and they are shifted toward the less electronegative atoms C1, C2 and C3. The O(1)-C(1), O(1)-C(2) and N(1)-C(1) bonds nearly equal to the value of topological parameters of N(1)-C(1) bond, the electron density = 3.3848, $\nabla^2\rho_b$(eÅ$^{-5}$) = -12.6587, $G_b$(he$^{-1}$) = 1.8135, $H_b$(he$^{-1}$) = -4.9781, $V$ = 6.7916, $\varepsilon_b$ = 0.1421. This is comparable with the reported pyridyl ligands. For instance, the N atom and C atom of pyridy ligand, $\rho_b$(eÅ$^{-3}$) = 3.386, $\nabla^2\rho_b$(eÅ$^{-5}$) = -10.578,
G_b(he^{-1}) = 2.203, H_b(he^{-1}) = -4.848, V = 7.051, \epsilon_b = 0.020 for N-C interactions of [Os_3(\mu-H)(\mu-\eta^2-dpa-N,N)(CO)]^-. That indicate the O(1)-C(1), O(1)-C(2), N(1)-C(1) and N(2)-C(1) bonds have a relatively smaller double bond character. These eye dances refers to found \pi-donation from the p-\pi orbitals of the N and O atoms to the empty p-\pi orbital of the C of d-\pi orbitals of metal carbene atom[33]. The topological parameter values of the oxazoline ligand, the highest electron density value, the most negative value of Laplacian, and the highest value of the ellipticity at bond critical points are consistent with the presence of double bond character within the oxazoline ring.

![Figure 8](image)

4. Conclusions

The chemical bonding in the triruthenium mono-hydride cluster [Ru_3(\mu^-H)(\mu_2-\kappa^2-Haminox-N,N)(CO)] is explored using the Quantum Theory of Atoms-in-Molecules (QTAIM). According to our calculations, we propose a multi-centre (5c–6e) type for the bridged core part (Ru_3H). As expected, the local topological parameters of the unbridged Ru–Ru bonds differ considerably from those of the bridged Ru…Ru bond, for which a bond path was not observed. A non-negligible delocalization indices \delta(Ru…Ru) was observed for the non-bonding interactions between Ru(1) and Ru(2). Topological parameters of Ru–N support for the presence of a \sigma-bond. In the oxazoline ligands, the analysis of the topological parameters of their bonds confirmed the existence of \pi-electron delocalization within the oxazoline ring.

The metal–metal and metal–ligand bond critical points properties and bond delocalization indices \delta(A, B) are aligned with the data from the previous studies on Os, Ru, Co, Fe, and Ni carbonyl complexes[29][21][8].

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