Characterization of $[\text{Rh}(\text{PhCOCHCOCH}_2\text{CH}_2\text{CH}_3)(\text{CO})_2]$ by X-ray crystallography, a computational and a statistical study

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Abstract

$[\text{Rh}(\text{PhCOCHCOCH}_2\text{CH}_2\text{CH}_3)(\text{CO})_2]$ is characterised by crystallographic and density functional theory computational methods. The experimental structure is compared to the calculated structure, as well as to the structurally similar compound $[\text{Rh}(\text{PhCOCHCOCH}_3\text{CH}_2)(\text{CO})_2]$ using root-mean-square calculations and a half-normal probability plot analyses.

1. Introduction

To compare two structures, we need a way to measure their similarities. The most widely-used geometrical similarity measure between two molecular structures is the Root-Mean-Square Deviation (RMSD) $^1$. There are also many other measures, but many of them are just variants of the RMSD $^2$. The RMSD is a metric used to assess the differences between the two molecular structures. It is defined as the square root of the minimum value of the average squared distance between each pair of corresponding atoms, over all the possible rotations and translations $^3$. A RMS-fit is the superposition of the structures that gives the smallest sum of squared distances between the related features. A RMS-fit thus provides a visual comparison, the minimized distances between individual atoms in two structures and a RMSD value. RMSD has successfully been used to determine the reliability of computational methods to give a good account of the experimental bonds and angles $^4$ and to give deeper insight into unique structures $^5$.

Half-normal probability (h.n.p.) plot analysis is a technique that has been successfully used to identify geometric differences between structures. In addition, the reliability of structural data can be evaluated using h.n.p. plot analysis $^6$. For example, in order to pinpoint the differences in geometry, h.n.p. plot analysis has been used to compare polymorphs $^7,^8$, concomitant polymorphs $^9$, different solvates of compounds (pseudo-polymorphs) $^10$ as well as isomorphous complexes $^11$. Half-normal probability plot analysis has also been used to compare a series of coordination compounds containing different anions $^12$. The influence of metal coordination on ligand geometry has also been identified using h.n.p. plot analyses $^13$.

In this work we present the structures of $[\text{Rh}(\text{PhCOCHCOCH}_3\text{CH}_2\text{CH}_3)(\text{CO})_2]$, 1, and $[\text{Rh}(\text{PhCOCHCOCH}_3\text{CH}_2\text{CH}_2\text{CH}_3)(\text{CO})_2]$, 2, by means of experimental X-ray structure and density functional theory (DFT) calculated geometries. We further validate the accuracy of the results by Root-Mean-Square fit and half-normal probability plot statistical methods.

2. Experimental

2.1. Crystallography

Crystals of 2 were grown from hot hexane at room temperature. Single crystal X-ray diffraction data for 2 were collected on a Bruker X8 Apex II 4K Kappa CCD diffractometer using Mo Kα (0.71073 Å) radiation with φ and ω-scans at 100(2) K. The initial unit cell and data collection were achieved by the $\text{APEX}^2$ $^14$ software utilizing COSMO $^15$ for optimum collection of the reciprocal space. All reflections were merged and integrated using $\text{SAINT}^16$ and were corrected for Lorentz, polarization and absorption effects using $\text{SADABS}^17$. The structures were solved by the direct method using $\text{SIR97}^18$ and refined through full matrix least-squares cycles using the $\text{SHELXL97}^19$ software package with $\Sigma[(\text{Fo})-|\text{Fc}|]^2$ being minimized. All non-H atoms were refined with anisotropic displacement parameters.
Aromatic and methyl H atoms were placed in geometrically idealized positions (C–H = 0.95 Å for aromatic and 0.98 Å for Me) and constrained to ride on their parent atoms, with \(U_{	ext{iso}}(H) = 1.2U_{	ext{eq}}(C)\) for aromatic and 1.5\(U_{	ext{eq}}(C)\) for methyl H atoms. The deepest residual electron-density hole (\(-0.54 \text{ e Å}^{-3}\)) is located at 0.87 Å from Rh, and the highest peak (0.63 \text{ e Å}^{-3}) 1.56 Å from H14. Crystal data and details of data collection and refinement are given in Table 1.

All structures were checked for solvent accessible cavities using PLATON [19] and the graphics were performed with the DIAMOND [20] Visual Crystal Structure Information System software.

### 2.2. Calculations

The accuracy of the computational approach was evaluated by comparing the root-mean-square distances (RMSDs) as calculated by the “RMS Compare Structures” utility in CHEMCRACK [21]. The RMSD values were calculated for the best three-dimensional superposition of optimized molecular structures on experimental crystal structures, using only the non-hydrogen atoms of the molecule. Data for the half-normal probability plots were processed using EXCEL2003 [22].

### 2.3. Computational details

DFT calculations were carried out using the ADF (Amsterdam Density Functional) 2009 program [23] with the GGA (Generalised Gradient Approximation) functional PW91 (Perdew–Wang, 1991) [24,25]. The TZP (Triplet \(\zeta\) polarised) basis set, with a fine mesh for numerical integration, a spin-restricted formalism and full geometry optimization with tight convergence criteria as implemented in the ADF 2009 program, was used. All calculations have been performed with no symmetry constraint (\(C_1\)) and all structures have been calculated as singlet states.

### 2.4. Synthesis

Complexes 1 and 2 were synthesized as described previously [26].

Characterization data for [Rh(PhCOCHCOCH2CH3)(CO)2], 1: M.p. 79–81 °C. IR (cm\(^{-1}\)) = 2065 and 2008. \(^1\)H NMR (\(\delta\)/ppm, CDCl\(_3\)): 1.2 (3H, t, CH3), 2.4 (2H, q, CH2), 6.2 (1H, s, CH) 7.4–7.9 (5H, m, C\(_2\)H\(_5\)). Elemental Anal. Calc. for RhC\(_2\)H\(_2\)O\(_2\): C, 46.7; H, 3.3. Found: C, 46.6; H, 3.1.

Characterization data for [Rh(PhCOCHCOCH2CH3)(CO)2], 2: M.p. 53–55 °C. IR (cm\(^{-1}\)) = 2084 and 2014. \(^1\)H NMR (\(\delta\)/ppm, CDCl\(_3\)): 1.0 (3H, t, CH3), 1.7 (2H, m, CH2), 2.4 (2H, t, CH2), 6.3 (1H, s, CH), 7.4–7.9 (5H, m, C\(_2\)H\(_5\)). Elemental Anal. Calc. for RhC\(_4\)H\(_3\)O\(_2\): C, 48.3; H, 3.8. Found: C, 48.2; H, 3.7.

### 3. Results and discussion

#### 3.1. Crystallography

A molecular diagram of both 1 and 2, showing atom labelling is presented in Fig. 1. Selected bond lengths and angles are given in Table 2. The structure of 1 was described previously [27], but is included here for comparative reasons. Comparative X-ray structural data with other [Rh(\(\alpha\)-diketonato)\((\text{CO})_2\)] are presented in Table 3.

The dicarbonyl complex 2 packs in the P1 space group with \(Z = 2\), resulting in molecules lying on general positions in their unit cells. The rhodium atom in both 1 and 2 has a nearly perfect square planar co-ordination sphere with the Rh atom displaced 0.040 and 0.030 Å respectively from the plane formed by four coordinating atoms. The bond angles in the rhodium polyhedron are within experimental error of the expected 90° for dsp\(^2\) hybridisation; however, deviations of up to 7° were found in the sp\(^2\) hybridised C atoms of the \(\beta\)-diketone skeleton, possibly due to strain from chelation with the metal. The phenyl rings of 1 and 2 forms a dihedral angle of 20.6° and 16.4° respectively with the pseudo aromatic core of the \(\beta\)-diketone ligand.

The Rh–O distances for both 1 and 2 are similar (ca. 2.03 Å), slightly shorter than in [Rh(C\(_2\)H\(_4\)COCHCOCH\(_2\)CH\(_3\))(CO)\(_2\)] (2.05 Å) [28,29] and slightly longer than in [Rh(C\(_6\)F\(_5\)COCHCOCH\(_2\)CH\(_3\))(CO)\(_2\)] (2.02 Å) [30]. The Rh–O distances are considered similar due to the standard deviation on complexes 1 and 2. This might be due to the similar electron donating properties of the CH\(_2\)H, Ph, CH\(_2\)CH\(_2\) and CH\(_2\)CH\(_2\)CH\(_2\) groups (the apparent group electronegativities, \(\chi\) of the R side group of the \(\beta\)-diketone is \(\chi_{\text{Ph}} = 2.21 [31], \chi_{\text{CH}} = 2.34 [32], \chi_{\text{CH} = 2.31, \chi_{\text{CH} = 2.41 and \chi_{\text{CH} = 2.22 on the Gordy scale [33]}. In [Rh(C\(_6\)F\(_5\)COCHCOCH\(_2\)CH\(_3\))(CO)\(_2\)] (see Table 3), however, the two Rh–O bonds differ slightly with ca. 0.03 Å, probably because of the stronger electron donating properties of the ferrocenyl \(\chi_{\text{Fer} = 1.87}\) compared to that of the CF\(_3\) group \(\chi_{\text{CF} = 3.01}\) on the \(\beta\)-diketone ligand FcCOCHCOCH\(_2\)F. All bond lengths and angles are in the typical range for these type of compounds (Table 3).

#### 3.2. DFT studies

Density functional theory computational methods have previously been shown to successfully optimize square planar rho-
medium(1) complexes, coordinated to a \( \beta \)-diketonato ligand [35]. Here we present the DFT optimized structures of 1 and 2 and compare it to the experimental structures, see Table 2 for selected data. A key indicator in organometallic compounds is the bond lengths and angles involving the metal centre. All bonds in the coordination polyhedron of 1 and 2 were slightly over-estimated (0.04 Å) by the DFT calculations (comparative information with signed deviations are given in Table S1, atom numbering is as indicated in Fig. 1). It is well-known that GGA density functionals overestimate bonds lengths [36] and that gas phase calculations give slightly longer bond lengths than corresponding crystal structure bond distances [37]. The angles around the Rh were calculated accurately within 0.4°. Since comparisons of experimental metal–ligand bond lengths with calculated bond lengths below a threshold of 0.02 Å are considered as meaningless, the methods employed in this study therefore give a good account of the experimental bond lengths of both 1 and 2.

### 3.3. Root-mean-square deviation calculations

The agreement between experimental and theoretical structures obtained, can also be expressed in terms of the RMSD values of the calculated data (all non-H atoms) superimposed on the experimental data, 0.057 and 0.391 Å for 1 and 2, respectively. The large RMSD value of 2 is due to the different orientation of the ethyl group in the experimental and the calculated structure. Fig. 2a, d, g give a visualization of the RMS-fit of the backbone (RhOCCCO) of experimental 1 on experimental 2, of calculated 1 on experimental 1 and of calculated 2 on experimental 2. The overlay plot of the backbone (RhOCCCO) of experimental 1 on experimental 2 of 0.027 vs. the RMSD of the non-H atoms of experimental 1 on experimental 2 of 0.406.

### 3.4. Half-normal probability plot analysis

Ordered weighted differences between matching parameters in independently determined structures follow a Gaussian distribu-

### Table 2

**Selected bond distances (Å) and angles (°) for 1 and 2.**

<table>
<thead>
<tr>
<th></th>
<th>1 (calculated)</th>
<th>2 (calculated)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bonds (Å)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Rh–C1</td>
<td>1.849(2)</td>
<td>1.880</td>
</tr>
<tr>
<td>Rh–C2</td>
<td>1.852(2)</td>
<td>1.880</td>
</tr>
<tr>
<td>Rh–O3</td>
<td>2.0288(13)</td>
<td>2.067</td>
</tr>
<tr>
<td>Rh–O4</td>
<td>2.0285(14)</td>
<td>2.066</td>
</tr>
<tr>
<td>O1–C1</td>
<td>1.133(2)</td>
<td>1.155</td>
</tr>
<tr>
<td>O2–C2</td>
<td>1.137(2)</td>
<td>1.155</td>
</tr>
<tr>
<td>Angles (°)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C1–Rh–C2</td>
<td>89.14(9)</td>
<td>89.5</td>
</tr>
<tr>
<td>C2–Rh–O4</td>
<td>89.87(7)</td>
<td>90.0</td>
</tr>
<tr>
<td>C1–Rh–O3</td>
<td>90.53(7)</td>
<td>90.0</td>
</tr>
<tr>
<td>O3–Rh–O4</td>
<td>90.36(6)</td>
<td>90.6</td>
</tr>
<tr>
<td>RMSD(^b, c)</td>
<td>– 0.057</td>
<td>– 0.391</td>
</tr>
</tbody>
</table>

\(^a\) Reference [27].

\(^b\) RMSD values, in Å, are root-mean-square atom positional deviations, calculated for the non-hydrogen atoms.

\(^c\) RMSD of experimental structure of 1 on the experimental structure of 2 is 0.406.

### Table 3

**Selected geometrical data from X-ray structures for [Rh(RCOCHCOR')\(\text{CO}_3\)] complexes.**

<table>
<thead>
<tr>
<th>Complex</th>
<th>C–Rh–C' (°)</th>
<th>Rh–O (Å)</th>
<th>Rh–O' (Å)</th>
<th>Rh–C (Å)</th>
<th>Rh–C' (Å)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Rh(CH$_3$COCHCOR')(\text{CO}_3)]</td>
<td>85</td>
<td>2.06</td>
<td>2.05</td>
<td>1.75</td>
<td>1.76</td>
<td>[28]</td>
</tr>
<tr>
<td>[Rh(CH$_3$COCHCOCH$_3$(\text{CO}_3)]</td>
<td>88.9(3)</td>
<td>2.044(4)</td>
<td>2.040(4)</td>
<td>1.831(7)</td>
<td>1.831(7)</td>
<td>[29]</td>
</tr>
<tr>
<td>[Rh((\text{PhCOCHCOCH}_3)(\text{CO}_3)]</td>
<td>89.14(9)</td>
<td>2.0285(14)</td>
<td>2.0288(13)</td>
<td>1.849(2)</td>
<td>1.852(2)</td>
<td>[27]</td>
</tr>
<tr>
<td>[Rh((\text{PhCOCHCOCH}_2\text{CH}_3)(\text{CO}_3)]</td>
<td>89.14(8)</td>
<td>2.0295(13)</td>
<td>2.0300(12)</td>
<td>1.851(2)</td>
<td>1.8446(19)</td>
<td>this work</td>
</tr>
<tr>
<td>[Rh(CF$_3$COCHCOPh)(\text{CO}_3)]</td>
<td>87(1)</td>
<td>2.02(2)</td>
<td>2.02(2)</td>
<td>1.79(3)</td>
<td>1.82(3)</td>
<td>[30]</td>
</tr>
<tr>
<td>[Rh(CF$_3$COCHCOFC)(\text{CO}_3)]</td>
<td>89.1(6)</td>
<td>2.059(4)</td>
<td>2.028(8)</td>
<td>2.8(4)</td>
<td>1.83(2)</td>
<td>[34]</td>
</tr>
</tbody>
</table>

\(^a\) Ph = phenyl.

\(^b\) Fc = ferrocenyl.
tion, only if both determinations are subject to the influence of random effects. Deviations from Gaussian are readily detectable by plotting experimental deviates against corresponding normal probability deviates – with a normal distribution (with an expectation of zero) producing a linear array of unit slope and zero intercept [38]. In 1973, De Camp suggested that inter-atomic distances can be used as chemical coordinates [39]. Half-normal probability (h.n.p.) plot analysis of the independently determined structures can be used to

(i). investigate the reliability of the standard uncertainties (s.u.’s) and
(ii). identify systematic geometrical differences in two molecules [40].

The h.n.p. plot analysis method consists of plotting the experimental deviates \( \delta m_i \), calculated using Eq. (1), versus the values \( a_i \) expected for a half-normal distribution of errors. The expected values \( (a_i) \) for normal and half-normal probability deviates are tabulated in the International Tables for X-ray crystallography [41].

\[
\delta m_i = \frac{|d(1)_i - d(2)_i|}{\sqrt{\sigma^2 d(1)_i + \sigma^2 d(2)_i}}
\]

(1)

The quantities \( d(1)_i \) and \( d(2)_i \) are inter-atomic distances for two different structures \( (1) \) and \( (2) \) with s.u.’s \( \sigma d(1)_i \) and \( \sigma d(2)_i \), respectively. When comparing computed structures with X-ray structures, we double the s.u.’s for the X-ray structure in formula 1, as the computed structures do not have any s.u.’s.

Using the h.n.p. plot analysis method, two different comparisons can be made:

(i). Using independent distances – distances chosen to represent a statistical sample.

(ii). Using dependent distances – representing atoms separated by one, two or three formal bonds.

The independent distances need to be analysed as a complete set. From the graph obtained by using independent distances, a slope and an intercept can be obtained by linear regression. A linear plot with a slope of unity and a zero intercept indicates a correct match between the compared sets of distances and correctly estimated s.u.’s. If the slope is larger (or smaller) than unity the s.u.’s are underestimated (or over-estimated). A non-linear plot, or a linear plot with a nonzero intercept, on the other hand, indicates systematic differences, which may be caused by either geometrical differences in the compared compounds or by systematic errors in the measurement procedure.

In contrast, the dependent distances are used to identify inter-atomic distances that are significantly different for the compared molecules and thus provide a quantitative companion for r.m.s. error calculations. The largest deviates \( (\delta m_i) \) for the dependent distances represent the largest geometric differences between the compared structures.

The backbones of the complexes studied contain 18 non-H atoms (Fig. S1 in the Supporting Information). Therefore 48 independent inter-atomic distances \( (3n - 6) \) completely describe the complex. To ensure a non-biased, statistical comparison only 48 dependent distances were used in the calculations. These dependent distances represent direct bond lengths (19; first order), bond angles (20; second order) and torsion angles (9; third order distances). Fig. 2 shows the h.n.p. plot of the 48 independent (Fig. 2b, e and h) and the 48 dependent (Fig. 2c, f and i) distances.

The independent distances for the comparison of \( 1 \) versus \( 2 \) (Fig. 2b) shows linear behaviour up to \( a_i = 1.2319 \), thus confirming a general similar geometry for \( 1 \) and \( 2 \), as well as indicating that no serious systematic mistakes are present. The major differences, as
expected, relate to the different position of C3 on the alkyl side group of the β-diketonato ligand. Linear regression resulted in a straight line (y = 3.98x – 0.31) showing that in general the s.u.’s of the compounds were underestimated with a factor of approximately 4, i.e. the s.u.’s should be four times larger than the reported ones. It is, however, a well reported fact that s.u.’s are generally underestimated by a factor of two to three (13a), however, a factor of up to seven is not unknown (1b).

The analysis of the dependent distances for the comparison of structure 1 versus 2 (Fig. 2c) confirmed the general similarity between the two compounds. Table 4 gives a summary of the inter-atomic distances with highest deviation of the calculated distances from the experimental structures, with a factor of approximately 1.5, i.e. the calculated distances should be about twice as large as the experimental ones. As expected, the biggest difference between the two structures is related to the different orientation of the alkyl group (C3 and C4). (The atom numbering used in the h.n.p. analysis (Fig. S1 in the Supporting Information) is according to the numbering of 1 in Fig. 1 (left)).

The h.n.p. analysis for the comparison of the calculated versus experimental structures (Fig. 2e, f, h, i) generally showed a remarkable resemblance between the calculated and experimental structures. The independent distance analysis (Fig. 2e and h) shows a general linear behaviour for all data-points except points related to the propyl carbons on 2. This is in agreement with the RMS-fit plot of 2 (Fig. 2g), visualizing the different orientations of the propyl sidegroup in the experimental crystal and the calculated structure of 2. As was found for the independent distances for the comparison of 1 versus 2 (Fig. 2b), the slopes of the independent distance analysis plots of experimental versus calculated (Fig. 2e and h) were larger than unity, indicating an underestimation of the s.u.’s. If we assume the underestimation of a factor of 4 for the s.u.’s, as found in the experimental comparison, we can determine from the plots of the independent distances that in general the calculated inter-atomic distances are 1.4% longer than the experimentally found ones. The inter-atomic distances are not over-estimated with a fixed amount as this leads to non-linear behaviour indicating that the geometry changes significantly. The longer inter-atomic distances for the calculated structures are the direct result of the calculations since gas phase calculations and GGA density functionals overestimate bonds lengths (also see Table S1).

The h.n.p. analysis of the dependent distances of the calculated versus experimental structures is shown in Fig. 2f and i. Fig. 2j, with s.u’s (C3–O4) = 86.1 clearly shows that the position of C3 in structure 2 is calculated to be different from the position in the X-ray structure. Additionally, the largest differences were found in the Rh–O distances (for both 1 and 2), indicating that the geometry around the Rh atom is modelled slightly differently. In general, however, an excellent agreement is found between the experimental X-ray structures and the theoretical modelled structures.

Overall, the results from the h.n.p. analysis confirm that (1) s.u.’s are underestimated in X-ray structures, and (2) inter-atomic bond distances are found to be longer in calculated structures than in X-ray structures. Other than these two major differences, we propose that half-normal probability plot analysis is an excellent tool for the validation of both X-ray structures and structures found by theoretical calculations, in agreement with RMSD calculations. Clearly, differences between two structures are immediately identified, and can be quantified, when using the h.n.p. statistical validation tools.

**Table 4**

**Interatomic distances with highest deviation of the calculated s.u. from expected statistical values x for 1 and 2 from Fig. 2c.**

<table>
<thead>
<tr>
<th>s.u.</th>
<th>Distance</th>
<th>Order*</th>
<th>Corresponding distances (Å) and [angles] (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>33.0</td>
<td>O4–C3</td>
<td>Third</td>
<td>2.880(3) [-51.8(3)]</td>
</tr>
<tr>
<td>11.4</td>
<td>C3–C5</td>
<td>Second</td>
<td>2.532(3) [113.48(19)]</td>
</tr>
<tr>
<td>6.4</td>
<td>O4–C4</td>
<td>Second</td>
<td>2.352(2) [114.49(17)]</td>
</tr>
<tr>
<td>5.1</td>
<td>Rh–C5</td>
<td>Second</td>
<td>2.968(2) [125.82(13)]</td>
</tr>
<tr>
<td>4.9</td>
<td>O3–C6</td>
<td>Second</td>
<td>2.383(2) [125.86(18)]</td>
</tr>
</tbody>
</table>

* First, second and third order refers to inter-atomic distances separated by one (bond distance), two (angles) and three (torsion angles) formal bonds, respectively.

**4. Conclusion**

The new compound 2 was synthesised and characterised. This compound is compared to the previously reported compound 1 using a combination of methods. Theoretical computations revealed a general similar structure of the two compounds. The h.n.p. analyses revealed that in general the s.u.’s are underestimated by a factor of 4. The generally similar geometry of 1 and 2, as well as both with their computed structures was confirmed by h.n.p. plot analyses. To the best of our knowledge this is the first time that computed and experimental structures are compared using h.n.p. plot analyses.

Both the h.n.p. plot analysis and Root-Mean-Square Deviation (RMSD) proof to be powerful tools to identify differences between structures i.e. pin-pointing which geometric parameters are the origin of the observed differences. Additionally the h.n.p. plot analysis is a tool to examine the reliability of experimental structural data if the s.u.’s are known. RMSD, however, can be used to compare any two sets of structural data for the same (or similar complexes) with only the xyz coordinates to be known.

**Acknowledgements**

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**Appendix A. Supplementary data**

CCDC 795253 contains the supplementary crystallographic data for [Rh(PhCOCH2COCH2CH2CH3)(CO)2]2. These data can be obtained free of charge via [http://www.ccdc.cam.ac.uk/conts/retrieving.html](http://www.ccdc.cam.ac.uk/conts/retrieving.html), or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk. Supplementary data associated with this article can be found, in the online version, at [doi:10.1016/j.poly.2010.11.038](http://doi.org/10.1016/j.poly.2010.11.038).
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