

Article

Predicting Pt-195 NMR Chemical Shift in Pt(II)-Sn(II) Complexes

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Abstract

Platinum chemistry covers a wide range of applications, including homogeneous and heterogeneous catalysis as well as cancer therapy. Numerous Pt complexes have been synthesized and studied in recent years, with NMR spectroscopy serving as the primary technique for structural characterization. The ¹⁹⁵Pt nucleus has favorable features for NMR studies, being highly sensitive to ligand type and structural environment. From a computational perspective, factors such as solvent effects, relativistic corrections, and the electronic structure of the ligands strongly influence the calculated NMR parameters. Consequently, establishing a general computational protocol for ¹⁹⁵Pt NMR prediction remains a challenging task. In this work, we present a systematic validation and extension of our previously developed computational protocol, originally proposed for Pt(II) complexes, in studying ¹⁹⁵Pt NMR chemical shifts in Pt(II)-Sn(II) complexes. A benchmark set of 100 Pt(II)-Sn(II) complexes was analyzed, yielding good agreement with experimental data ($R^2 = 0.86$, MRD = 3.6%, MAD = 163 ppm), which is remarkable given the structural diversity and broad range of chemical shifts covered.

Keywords: catalysts; Pt(II)-Sn(II) complexes; Pt-195 NMR; computational protocol; NMR-DKH basis set

1. Introduction

Platinum chemistry encompasses a wide range of applications, including heterogeneous catalysts for automobile exhaust treatment, homogeneous catalysts for organic synthesis, and potential anticancer drugs [1–7]. In catalysis, Pt(II) complexes coordinated with Sn(II) are recognized as highly efficient homogeneous catalysts for hydrogenation, hydroformylation, carbonylation, and dehydrogenation reactions [8–15]. These complexes exhibit remarkable activity for C–H bond activation and a low propensity for C–C bond cleavage, offering significant advantages over the Rh- and Co-based catalysts widely used in industry [9,10,16]. A representative example is the conversion of acetic acid to ethanol, where Pt–Sn catalysts promote direct ethanol formation with high selectivity [17].

Pentacoordinate complexes of Pt(II) and Sn(II) were first investigated in 1964. The main species of interest was $[\text{Pt}(\text{SnCl}_3)_5]^{3-}$, characterized by a central Pt(II) atom coordinated by five SnCl_3^- ligands [18]. This complex highlighted the importance of strong *trans* activation in both catalytic activity and ligand exchange reactions [19]. Notably, $[\text{Pt}(\text{SnCl}_3)_5]^{3-}$ is one of the few species capable of catalyzing the hydrogenation of ethylene and acetylene



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under mild conditions, and it can serve either as a catalyst or as a precursor in reactions such as vinyl halide coupling and styrene hydrogenation [12,20]. Later, in 1984, Pregosin and Ruegger studied Pt and Pd salts with excess Sn(II) chloride. From their NMR spectra, new complexes containing SnCl_3^- ligands were identified and recognized as effective homogeneous hydrogenation catalysts [11].

The ^{195}Pt nucleus is the only NMR-active platinum isotope and possesses several favorable properties ($I = 1/2$, $\gamma(^{195}\text{Pt}) = 5.768 \times 10^7 \text{ rad s}^{-1} \text{ T}^{-1}$, resonance frequency 64.5 MHz at 7.05 T, natural abundance of 33.8%, relative sensitivity 0.00994 vs. $^1\text{H} = 1.00$, and absolute sensitivity 0.00336). In addition, its chemical shift ($\delta^{195}\text{Pt}$) is highly sensitive to conformation, oxidation state, and molecular environment. The chemical shift range for ^{195}Pt is unusually large, spanning approximately 15,000 ppm (from +8000 to −7000 ppm) relative to the reference compound $[\text{PtCl}_6]^{2-}$ [21,22]. The relevance of Pt(II)-Sn(II) complexes in homogeneous catalysis, combined with the attractive spectroscopic properties of ^{195}Pt , makes ^{195}Pt NMR an important analytical tool [23]. Moreover, NMR plays a fundamental role in elucidating reaction mechanisms [24].

The theoretical prediction of ^{195}Pt NMR chemical shifts can provide support to experimental studies of Pt(II)-Sn(II) complexes. However, this task is far from trivial, as the computed values are strongly influenced by many factors, including solvent effects, relativistic contributions, and the geometry and electronic structure of the coordinated ligands. Gilbert and Ziegler [25] showed that calculations employing DFT with the inclusion of relativistic effects in predicting the $\delta^{195}\text{Pt}$ in neutral PtX_2L_2 type compounds showed good agreement with experimental data. The importance of including solvent effects (implicit/explicit) for an adequate description of $\delta^{195}\text{Pt}$ is well explored in the literature [26–30]. Gabano et al. [31] employed a chemometric approach using an artificial neural network algorithm in 185 Pt(II) complexes with good agreement with experimental data. Models using machine learning have also been successfully employed in the study of ^{195}Pt NMR [32,33]. Studies employing relativistic four-component calculations were performed by Semenov et al. [34,35]. On the other hand, Tsipis and Karapetsas calculated $\delta^{195}\text{Pt}$ with good agreement with experimental data using nonrelativistic Hamiltonians [36–39].

Despite several studies addressing the prediction of $\delta^{195}\text{Pt}$, computational studies of Pt(II) complexes with direct Pt-Sn bonding are scarce, even with rich experimental literature on ^{195}Pt NMR in Pt-Sn compounds.

Paschoal et al. [40] developed an effective nonrelativistic computational protocol to predict $\delta^{195}\text{Pt}$ shifts for Pt(II) complexes. To partially recover relativistic effects, the authors constructed a dedicated Gaussian basis set, named NMR-DKH, for Pt and all ligand atoms. The $\delta^{195}\text{Pt}$ values were obtained using an empirical model based on the linear correlation between experimental $\delta^{195}\text{Pt}$ chemical shifts and the corresponding calculated shielding constants ($\sigma^{195}\text{Pt}$). The $\sigma^{195}\text{Pt}$ values were computed at the GIAO-PBE/NMR-DKH/IEF-PCM(UFF)//B3LYP/LANL2DZ/def2-SVP/IEF-PCM(UFF) level of theory, where geometries were optimized at B3LYP/LANL2DZ/def2-SVP/IEF-PCM(UFF) and shielding constants were calculated at GIAO-PBE/NMR-DKH/IEFPCM(UFF). This protocol was applied to a dataset of 258 Pt(II) complexes (with 183 used as the training set and 75 used as the external validation set), and yielded a mean relative deviation (MRD) of only 5% and a mean absolute deviation (MAD) of 168 ppm with respect to experimental data. Among the 258 complexes, only two contained Sn(II) ligands: *trans*- $[\text{PtCl}(\text{SnCl}_3)(\text{PEt}_3)_2]$ (MRD = 0.4%, MAD = 100 ppm) and *trans*- $[\text{PtH}(\text{SnCl}_3)(\text{PEt}_3)]$ (MRD = 0.5%, MAD = 126 ppm).

Recently, Kondrashova and Latypov [41] evaluated different DFT functionals, basis sets, and the inclusion of relativistic effects in predicting $\delta^{195}\text{Pt}$ in Pt(II) and Pt(IV) complexes. The results obtained by the authors showed that the NMR-DKH basis set is

particularly suitable for studying the ^{195}Pt NMR, since it presents a better description of the electron density in the core region.

Considering the multiple factors that strongly influence ^{195}Pt NMR, the theoretical prediction of $\delta^{195}\text{Pt}$ chemical shifts remains an extremely challenging task, highlighting the need for a robust and general computational protocol. In this context, the present work applies our previously proposed nonrelativistic protocol [40] to Pt(II)-Sn(II) complexes, with the aim of evaluating and validating its performance in predicting $\delta^{195}\text{Pt}$ shifts for a representative set of complexes containing Pt-Sn bonds.

2. Methodology

A set of 100 Pt(II)-Sn(II) complexes for which experimental $\delta^{195}\text{Pt}$ chemical shifts are available was selected [11,22,42–50]. The geometries of these complexes were optimized and characterized as minima on the potential energy surface (PES) at the B3LYP/LANL2DZ/def2-SVP/IEFPCM(UFF) level of theory. This approach combines the hybrid DFT functional B3LYP [51–53] with the LANL2DZ effective core potential (ECP, 60 electrons) and corresponding valence basis set for Pt [54], and the def2-SVP basis set for the ligand atoms [55,56]. It is important to note that the def2-SVP basis set for Sn also includes an ECP for the 28 core electrons [55]. Solvent effects on both the geometry and the NMR calculations were incorporated using the IEF-PCM (Integral Equation Formalism for the Polarizable Continuum Model) with atomic radii set according to the UFF (Universal Force Field) [57]. The solvents employed in the experimental NMR measurements were considered in the calculations. All geometry optimizations were carried out with the GAUSSIAN 16 Rev. C.01 program [58].

For the complexes $[\text{Pt}(\text{SnCl}_3)_5]^{3-}$ (Cpx39) [59] and *trans*- $[\text{Pt}(\text{COC}_6\text{H}_5)(\text{SnCl}_3)(\text{PEt}_3)_2]$ (Cpx61) [50] (Figure 1), experimental X-ray structures are available in the literature. These structures were therefore used as benchmarks to assess the performance of the computational protocol in predicting the geometries of Pt(II)-Sn(II) complexes.

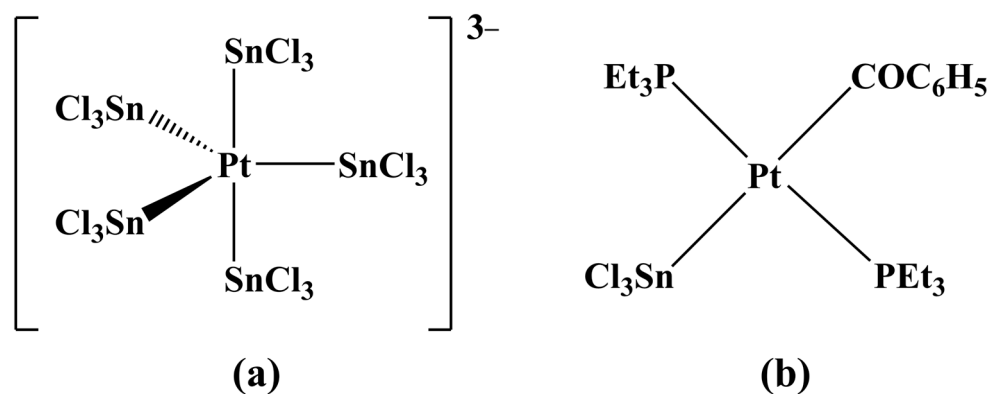


Figure 1. Pt(II)-Sn(II) complexes with experimental X-ray diffraction data available. (a) $[\text{Pt}(\text{SnCl}_3)_5]^{3-}$ (Cpx39) [59] and (b) *trans*- $[\text{Pt}(\text{COC}_6\text{H}_5)(\text{SnCl}_3)(\text{PEt}_3)_2]$ (Cpx61) [50]. Straight lines represent bonds in the plane of the page; solid wedges represent bonds projecting out of the plane toward the observer, whereas hashed wedges represent bonds projecting behind the plane.

The $\delta^{195}\text{Pt}$ chemical shifts were calculated using Equation (1), where $\sigma^{195}\text{Pt}$ represents the shielding constant obtained with the GIAO (Gauge-Independent Atomic Orbital) [60–64] approximation at the PBE/NMR-DKH/IEF-PCM(UFF) level of theory. This approach combines the GGA DFT functional PBE [65,66] with the NMR-DKH basis

set, which is an all-electron basis set specifically designed for all atoms, with particular emphasis on accurately describing NMR properties [40,67–72].

$$\delta^{195}\text{Pt} = -2065.7558 - 0.9250\sigma^{195}\text{Pt} \quad (1)$$

The NMR properties were calculated using the GAUSSIAN 16 Rev. C.01 program [58].

3. Results and Discussion

3.1. Structural Analysis

The geometries of the complexes $\text{Cpx39}[\text{Pt}(\text{SnCl}_3)_5]^{3-}$ and $\text{Cpx61-}trans\text{-}[\text{Pt}(\text{COC}_6\text{H}_5)(\text{SnCl}_3)(\text{PEt}_3)_2]$ were optimized and characterized as a minimum point on the PES (all harmonic frequencies found real) at B3LYP/LANL2DZ/def2-SVP/IEF-PCM(UFF) level (Figure 2). Calculated bond lengths and angles were compared to the solid-state X-ray structures [50,59] (Table 1).

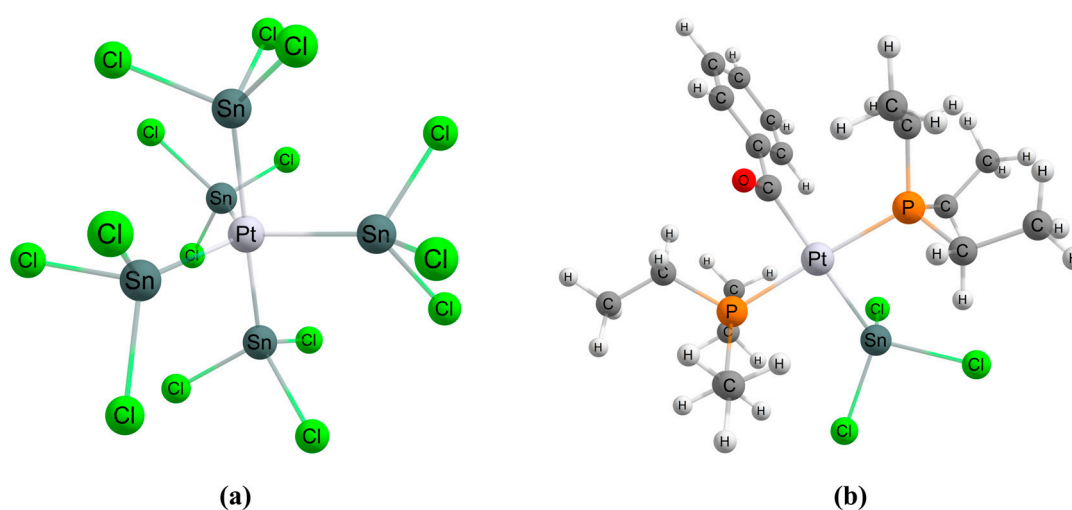


Figure 2. Optimized structures for the Pt(II)-Sn(II) complexes. (a) $\text{Cpx39}[\text{Pt}(\text{SnCl}_3)_5]^{3-}$, (b) $\text{Cpx61-}trans\text{-}[\text{Pt}(\text{COC}_6\text{H}_5)(\text{SnCl}_3)(\text{PEt}_3)_2]$. The level of theory employed was B3LYP/LANL2DZ/def2-SVP/IEF-PCM(UFF).

Table 1. Bond lengths (in Å) and bond angles (in degrees) for the complexes $\text{Cpx39}[\text{Pt}(\text{SnCl}_3)_5]^{3-}$ and $\text{Cpx61-}trans\text{-}[\text{Pt}(\text{COC}_6\text{H}_5)(\text{SnCl}_3)(\text{PEt}_3)_2]$ obtained at the level B3LYP/LANL2DZ/def2-SVP/IEF-PCM(UFF). The experimental X-ray data are also included.

$\text{Cpx39}[\text{Pt}(\text{SnCl}_3)_5]^{3-}$	Calc.	Expt. [59]	RD ^a
Pt-Sn (axial)	2.64	2.55	3.7%
Pt-Sn (equatorial)	2.70	2.57	5.0%
Sn-Pt-Sn (axial)	179.5	180.0	0.3%
Sn-Pt-Sn (equatorial)	120.0	120.0	0.0%
MRD ^b			2.2%
$\text{Cpx61-}trans\text{-}[\text{Pt}(\text{COC}_6\text{H}_5)(\text{SnCl}_3)(\text{PEt}_3)_2]$	Calc.	Expt. [50]	RD ^a
Pt-Sn	2.79	2.63	6.1%
Pt-P	2.40	2.32	3.4%
Pt-C	2.04	2.05	0.5%
P-Pt-P	173.8	170.8	1.8%
C-Pt-Sn	171.9	173.1	0.7%
P-Pt-C	90.9	90.3	0.7%
P-Pt-Sn	90.3	92.2	2.1%
MRD ^b			2.2%

^a RD = relative deviation; ^b MRD = mean relative deviation.

For Cpx39, the calculated Pt-Sn(axial) and Pt-Sn(equatorial) bond lengths showed relative deviations (RD) of 3.7% and 5.0%, respectively. In contrast, the bond angles were less sensitive, with Sn-Pt-Sn(equatorial) and Sn-Pt-Sn(axial) angles showing RD of only 0.3% and 0.0%. For Cpx61, which contains Pt-Sn, Pt-C, and Pt-P bonds in the coordination sphere, the RD were 5.8%, 0.3%, and 3.3%, respectively. The corresponding bond angles (P-Pt-P, C-Pt-Sn, P-Pt-C, and P-Pt-Sn) showed deviations below 2.5%. Overall, the MRD across all structural parameters was 2.2% for both complexes. Most of the deviation is due to the Pt-Sn bond, which was consistently overestimated. These results demonstrate that the theoretical level used for geometry optimization provides a reliable description of Pt(II)-Sn(II) complex structures. It is important to note that some differences are expected, as the calculations represent solution-phase structures (continuous model), whereas the experimental data are obtained in a solid state.

3.2. Calculation of $\delta^{195}\text{Pt}$

Equation (1) was first applied to predict the $\delta^{195}\text{Pt}$ chemical shifts of complexes Cpx39 and Cpx61, where the shielding constant ($\sigma^{195}\text{Pt}$) was calculated at the GIAO-PBE/NMR-DKH/IEF-PCM(UFF) level of theory. In these calculations, the all-electron NMR-DKH basis set was employed for all atoms. The predicted values were -5916 ppm and -4460 ppm, respectively, both in excellent agreement with the experimental data (-5894 ppm [11] and -4532 ppm [50]). Next, we applied the same computational protocol to a broader set of Pt(II)-Sn(II) complexes for which experimental data are available (Table S1).

The experimental shifts range from -2748 to -5894 ppm and show a strong correlation with the predicted values (Figure 3), with the regression explaining about 86% of the variance ($R^2 = 0.86$). Statistical analysis further indicates a mean absolute deviation (MAD) of 163 ppm, corresponding to a mean relative deviation (MRD) of only 3.6%. The largest deviation was found for $[\text{PtClAsEt}_3](\mu\text{-Cl})_2[\text{Pt}(\text{SnCl}_3)\text{AsEt}_3]$ (20.1%), $[\text{PtCl}_3(\text{SnCl}_3)_2]^-$ (17.6%), followed by $[\text{Pt}(\text{SnCl}_3)_3(\text{P}(\text{OPh})_3)_2]^-$ (12.7%), *cis*- $[\text{PtCl}_2(\text{SnCl}_3)_2]^{2-}$ (11.8%), *cis*- $[\text{Pt}(\text{SnPh}_2(\text{SCH}_2\text{Ph}))\text{Ph}(\text{PPh}_3)_2]$ (11.8%), and $[\text{PtClPEt}_3](\mu\text{-Cl})_2[\text{Pt}(\text{SnCl}_3)\text{PEt}_3]$ (11.1%). For the remaining 94 complexes, the absolute RD was below 10%, demonstrating that the computational protocol is robust and applicable to a broad set of Pt(II)-Sn(II) complexes.

When a direct comparison between calculated and experimental values is performed (Figure 4), good agreement is observed for most complexes. To better assess the reliability of the computational protocol, the dataset was divided into groups according to their net charge (0, -1 , -2 , and -3 ; see Table S1). For neutral complexes (81 compounds), the MRD was 3.2%, increasing to 4.7% for anionic complexes with charge -1 (12 compounds) and 8.5% for those with charge -2 (5 compounds). For the group with net charge -2 , the calculated $\delta^{195}\text{Pt}$ values are generally more negative than the experimental values, indicating that the ^{195}Pt nucleus is more shielded than observed experimentally. The larger MRD observed for these complexes can therefore be attributed, at least in part, to counterion effects that were not included in original protocol and consequently in the calculations of the present work. By contrast, the two complexes with charge -3 were satisfactorily described by the computational protocol, with RD values below 2.5%.

Tsipis et al. [37,38] showed that in solution, ion-pairing interactions between charged complexes and their counterions can result in changes in the geometry and electronic structure around the coordination sphere of the Pt nucleus, which would result in changes in the calculated $\delta^{195}\text{Pt}$ values. In order to evaluate the effect of the counterion on Pt(II)-Sn(II) anionic complexes, the computational protocol was applied to the study of these complexes with the explicit inclusion of counterions.

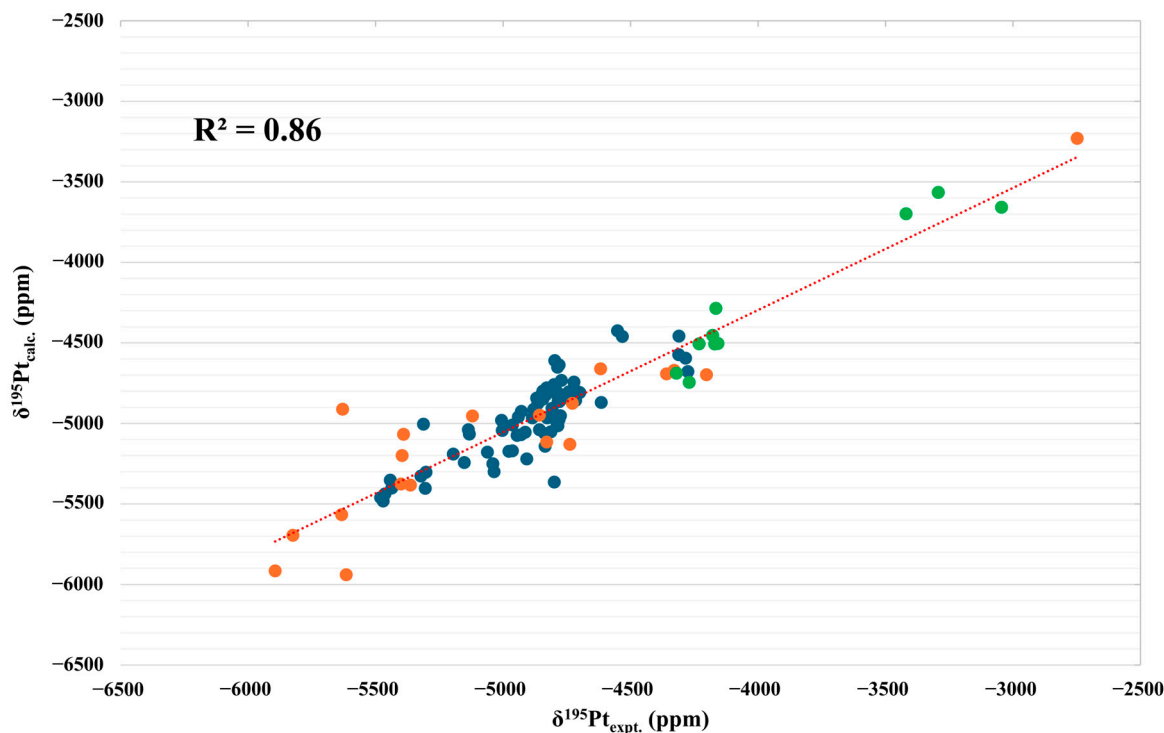


Figure 3. Correlation between the calculated and experimental values of $\delta^{195}\text{Pt}$ for 100 Pt(II)-Sn(II) complexes. Charged complexes are highlighted in orange, bimetallic complexes in green, and other complexes in blue.

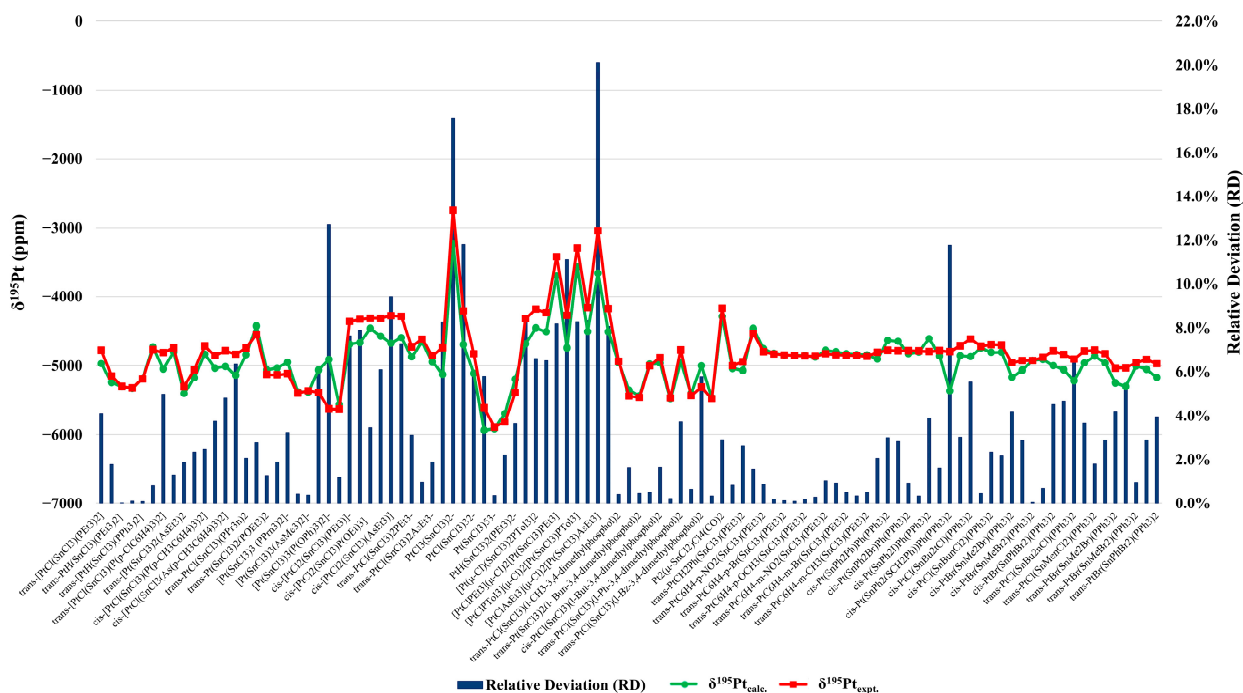


Figure 4. Comparison between the calculated (green line) and experimental (red line) $\delta^{195}\text{Pt}$ values for the 100 Pt(II)-Sn(II) complexes studied. The relative deviation (RD) is shown as blue bars. $\delta^{195}\text{Pt}$ values are displayed on the left vertical axis, while RD values are plotted on the right vertical axis.

From the calculated results (Figure 5 and Table S2), it can be seen that the inclusion of counterions results in small variations in the calculated $\delta^{195}\text{Pt}$, with variations of around 20 to 300 ppm being observed. Despite the variations, the general trends observed in the calculated $\delta^{195}\text{Pt}$ remain the same when the counterions are included, with the experimentally

observed trend being adequately described with and without the inclusion of counterions. These results indicate that the computational protocol employed can recover the electronic effects that influence the shielding of the ^{195}Pt nucleus in Pt(II)-Sn(II) complexes. It should also be kept in mind that the applied protocol was not constructed with the inclusion of counterion effects in the charged complexes.

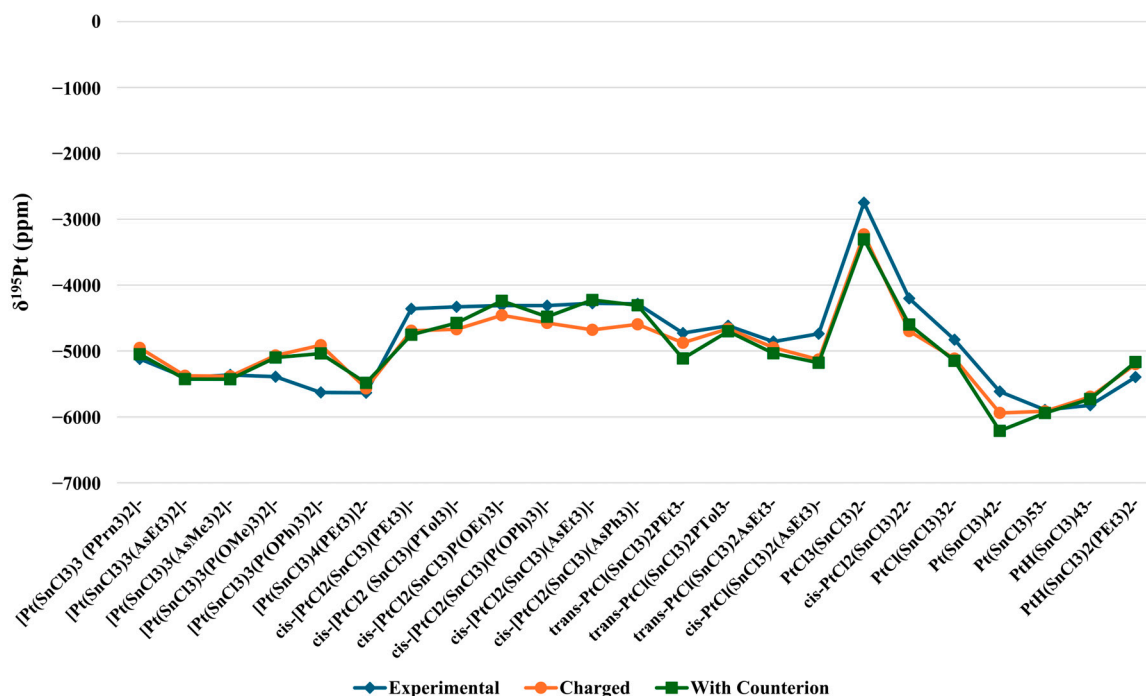


Figure 5. Comparison between the experimental and calculated with (MRD = 5.2%) and without (MRD = 5.5%) the inclusion of counterions $\delta^{195}\text{Pt}$ values for the charged Pt(II)-Sn(II) complexes studied.

When the subset of complexes containing two Pt centers is considered (7 complexes with 10 signals; see Table S3), the MRD increases to 8.7%. This higher deviation can be attributed to stronger relativistic effects arising from the presence of two Pt nuclei. However, it is observed that the calculated values adequately describe the experimentally observed trends.

The complexes were also analyzed with respect to the number of SnCl_3^- ligands, which ranged from one to five (see Table S4). It can be observed that the values of $\delta^{195}\text{Pt}$ vary between -2748 and -5322 ppm for one SnCl_3^- ligand, -4178 and -5480 ppm for two ligands, -4829 and -5629 ppm for three ligands, -5615 and -5824 ppm for four ligands, and -5894 ppm for five ligands. The observed trends in $\delta^{195}\text{Pt}$ values can also be qualitatively interpreted in terms of ligand electronic effects. In general, stronger σ -donor ligands increase electron density at the platinum center, leading to increased shielding and therefore more negative $\delta^{195}\text{Pt}$ values. The presence of SnCl_3^- ligands significantly influences the Pt electronic environment due to their strong *trans* influence and σ -donor character, which contributes to the large shielding observed for many complexes.

In general, the MRD increased with the number of SnCl_3^- ligands, except for the complexes containing four or five ligands. For complexes with one SnCl_3^- ligand (42 compounds with 45 signals), the MRD was 4.0%, being 2.9% without the three bimetallic complexes that presented the highest RD in this series. The MRD increased to 3.4% for complexes with two ligands (19 complexes) and to 4.8% for complexes with three ligands (6 compounds). In contrast, the MRD values were lower for complexes containing four and five SnCl_3^- ligands, 3.1% (3 compounds) and 0.4% (1 compounds), respectively. Overall,

the increase in MRD can be attributed to the higher negative charge generally associated with a greater number of SnCl_3^- ligands, as well as to stronger relativistic effects resulting from the increasing number of Pt-Sn bonds.

The nature of the ligand *trans* to the SnCl_3^- group also influences the $\delta^{195}\text{Pt}$. A clear trend can be observed for the series *trans*- $[\text{PtX}(\text{SnCl}_3)(\text{PEt}_3)_2]$, where X (COC_6H_5^- , Cl^- , CH_2Ph^- , CH_3^- , SnCl_3^- , and H^-) represents different ligands coordinated to platinum. The $\delta^{195}\text{Pt}$ values (Figure 6) become progressively more negative as the σ -donor strength of the ligand increases. For example, the acyl ligand COC_6H_5^- , which has significant π -acceptor character, leads to the least negative chemical shift (−4532 ppm), indicating reduced shielding at the Pt nucleus. In contrast, strongly σ -donating ligands such as hydride (H^-) and SnCl_3^- produce substantially more negative chemical shifts (−5302 and −5152 ppm, respectively), reflecting increased electron density at the Pt center. Alkyl ligands such as CH_3^- and CH_2Ph^- show intermediate behavior, consistent with their strong σ -donor but weak π -acceptor character. This trend demonstrates that the computational protocol can reproduce subtle electronic effects associated with ligand donor properties.

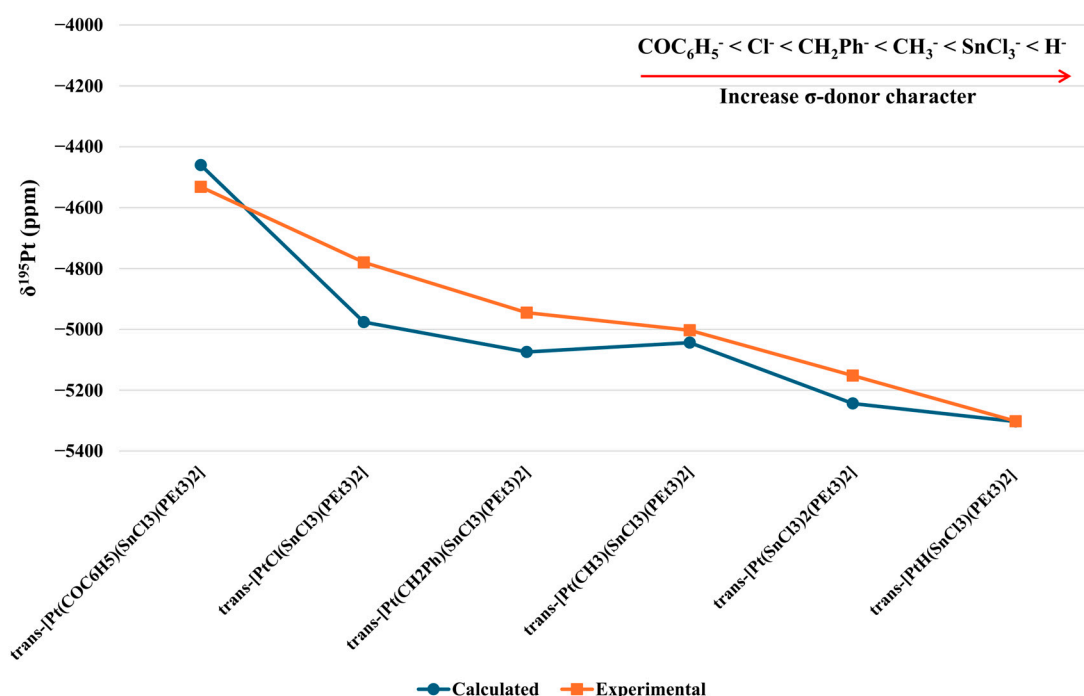


Figure 6. Assessment of nature of the ligand *trans* to the SnCl_3^- in the $\delta^{195}\text{Pt}$ chemical shift values for the series *trans*- $[\text{PtX}(\text{SnCl}_3)(\text{PEt}_3)_2]$, where X = COC_6H_5^- , Cl^- , CH_2Ph^- , CH_3^- , SnCl_3^- , and H^- .

Lastly, nine of the complexes studied present coordination number (CN) = 5, adopting trigonal bipyramidal geometry (see Table S5). For this subset, the MRD was 3.4%. Although the computational protocol was originally developed for Pt(II) complexes with CN = 4 and square-planar geometry, the MRD obtained for these nine complexes is of the same order as the average of the full dataset (3.6%). The similar level of accuracy observed for four- and five-coordinate complexes suggests that the protocol captures the main electronic factors governing the ^{195}Pt shielding in these systems. This finding also indicates that the method may be applicable to a broader range of Pt(II) coordination geometries, which may be largely attributed to the use of the all-electron NMR-DKH basis set for Pt and the coordinating ligand atoms.

Finally, a subset of structurally related complexes was selected to evaluate the ability of the computational protocol to distinguish subtle structural differences. Figure 7 shows the series of complexes with general formula *trans*- $[\text{Pt}(\text{C}_6\text{H}_4\text{-m-L})(\text{SnCl}_3)(\text{PEt}_3)_2]$,

where L = Br, OCH₃, or CH₃. The experimental $\delta^{195}\text{Pt}$ values for this series range from -4851 ppm (L = Br) to -4868 ppm (L = CH₃). The calculated $\delta^{195}\text{Pt}$ values were -4827 ppm (L = Br), -4839 ppm (L = OCH₃), and -4843 ppm (L = CH₃). The experimental variation in chemical shift across the three complexes was 17 ppm, while the calculated variation was 16 ppm. Moreover, the computational protocol correctly reproduced the experimental trend, confirming its ability to capture subtle substituent effects on $\delta^{195}\text{Pt}$.

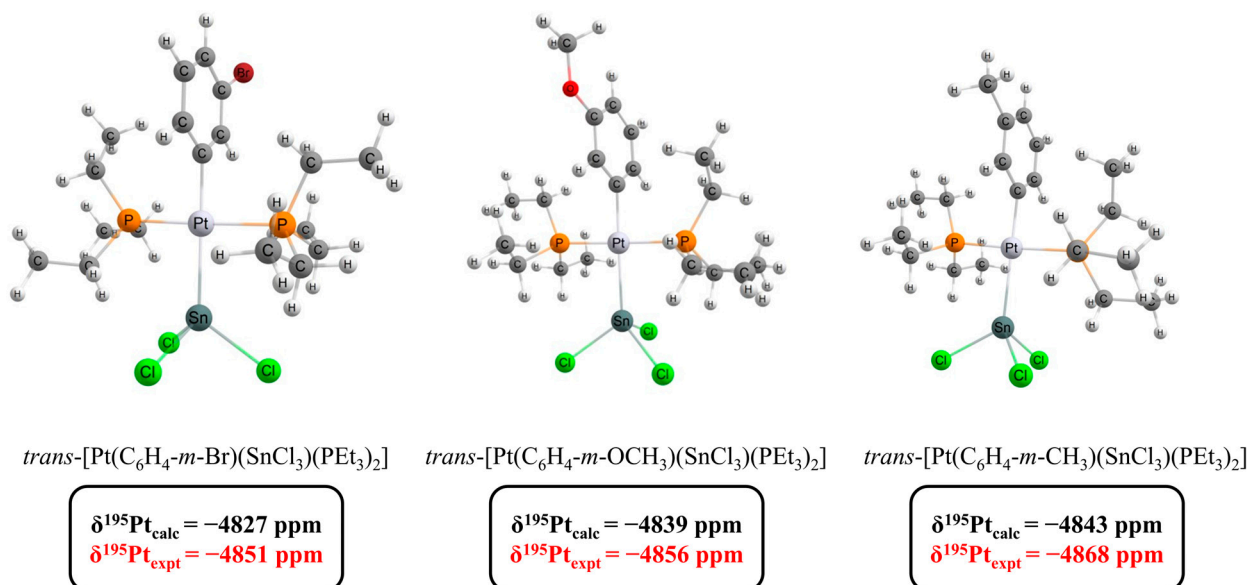


Figure 7. Comparison of the $\delta^{195}\text{Pt}$ chemical shift of the three compounds with a *trans*-[Pt(C₆H₄-*m*-L)(SnCl₃)(PEt₃)₂] profile of L = Br, OCH₃ and CH₃.

A comparison was also performed for the complexes with general formula *trans*-[PtH(SnCl₃)(PL)₂], where L = Et₃, Ph₂CH₂Ph, or Ph₃ (Figure 8). These species differ only in the nature of the phosphine ligands, leading to experimental $\delta^{195}\text{Pt}$ values ranging from -5302 ppm (L = Et₃) to -5195 ppm (L = Ph₃). The calculated values reproduced the experimental trends with high accuracy, with the largest absolute deviation being only 5 ppm for the complex with L = Ph₂CH₂Ph.

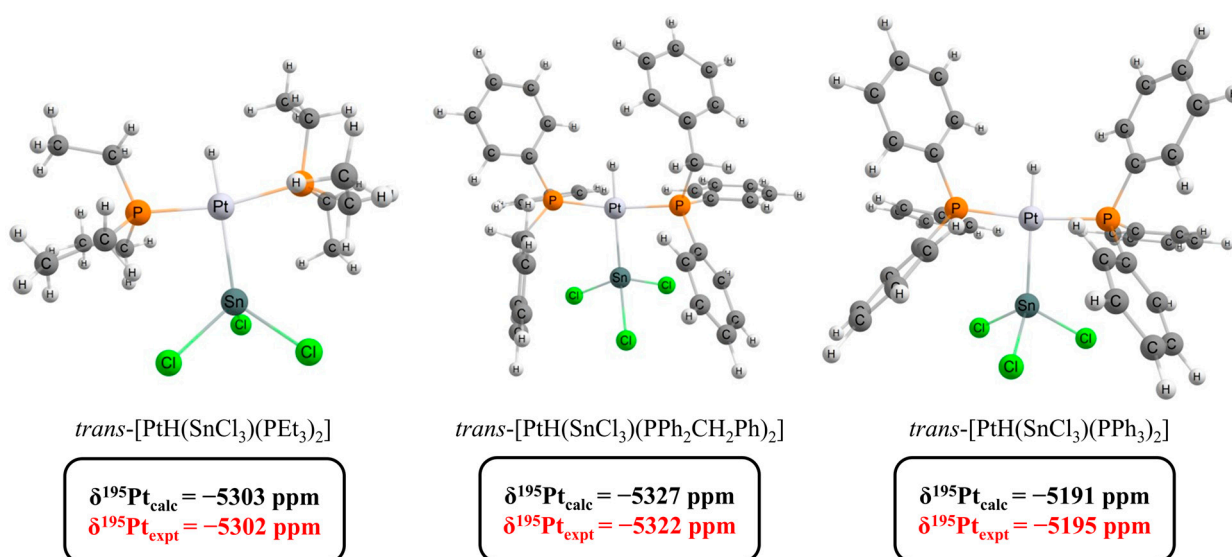


Figure 8. Comparison of the chemical shift of the three compounds with *trans*-[PtH(SnCl₃)(PL)₂] molecular formula with L = Et₃, Ph₂CH₂Ph e Ph₃.

In summary, the computational protocol previously proposed for Pt(II) complexes [30], satisfactorily reproduced the $\delta^{195}\text{Pt}$ chemical shifts of Pt(II)-Sn(II) complexes. Furthermore, the protocol was sensitive enough to distinguish subtle variations in ligand environments, making it a reliable and practical tool for assigning ^{195}Pt NMR spectra of these complexes.

4. Conclusions

In this work, the ^{195}Pt chemical shifts were calculated for a set of 100 Pt(II)-Sn(II) complexes (103 $\delta^{195}\text{Pt}$). The computational protocol employed was previously developed for Pt(II) complexes and incorporated our custom basis set for NMR predictions, named NMR-DKH. The protocol consisted of three steps: (i) geometry optimization at the B3LYP/LANL2DZ/def2-SVP/IEF-PCM(UFF) level; (ii) calculation of shielding constants ($\sigma^{195}\text{Pt}$) at the GIAO-PBE/NMR-DKH/IEF-PCM(UFF) level; and (iii) determination of $\delta^{195}\text{Pt}$ values from a linear scaling relationship: $\delta^{195}\text{Pt} = -2065.7558 - 0.9250\sigma^{195}\text{Pt}$.

The first part of the protocol was evaluated using two probe complexes for which experimental X-ray structures were available: $[\text{Pt}(\text{SnCl}_3)_5]^{3-}$ (Cpx39) and *trans*- $[\text{Pt}(\text{COC}_6\text{H}_5)(\text{SnCl}_3)(\text{PET}_3)_2]$ (Cpx61). The mean relative deviation (MRD) for both complexes was 2.2%, with most of the discrepancy arising from the Pt-Sn bond lengths, which were predicted to be ~6% longer than observed experimentally.

For the NMR analysis, $\delta^{195}\text{Pt}$ values were calculated for 100 complexes with experimental shifts ranging from -2748 ppm to -5894 ppm. The computed values showed satisfactory agreement with experimental values, with $R^2 = 0.86$, $\text{MAD} = 163$ ppm, and $\text{MRD} = 3.6\%$. Among these, 26 complexes exhibited $\text{MRD} > 5\%$, and only 6 had $\text{MRD} > 10\%$. Part of the deviation can be attributed to the increase in negative charge: the MRD was 3.2% for neutral complexes, rising to 4.7% and 8.5% for complexes with net charges of -1 and -2 , respectively. Complexes containing two Pt nuclei also showed deviations above the average ($\text{MRD} = 8.7\%$), suggesting more pronounced relativistic effects that are not fully captured by the current protocol. Nevertheless, the methodology proved capable of distinguishing subtle differences between isomers of Pt(II)-Sn(II) complexes.

Overall, the NMR-DKH basis set combined with the computational protocol previously proposed for Pt(II) complexes provides a reliable approach for predicting $\delta^{195}\text{Pt}$ in Pt(II)-Sn(II) complexes and demonstrates that it may serve as a practical computational tool for future studies of Pt coordination chemistry, including octahedral Pt(IV) complexes.

Supplementary Materials: The following supporting information can be downloaded at <https://www.mdpi.com/article/10.3390/magnetochemistry12040049/s1>: Tables S1–S5 provide molecular formulas, NMR data, and classification of complexes by net charge, counterions, Pt content, number of SnCl_3^- ligands, and Pt coordination number 5.

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References

- Gandhi, H.S.; Graham, G.W.; McCabe, R.W. Automotive Exhaust Catalysis. *J. Catal.* **2003**, *216*, 433–442. [\[CrossRef\]](#)
- Omrani, M.; Gorlaux, M.; Liu, Y.; Martinet, S.; Jean-Soro, L.; Ruban, V. Platinum Group Elements Study in Automobile Catalysts and Exhaust Gas Samples. *Environ. Pollut.* **2020**, *257*, 113477. [\[CrossRef\]](#)
- Meister, T.K.; Riener, K.; Gigler, P.; Stohrer, J.; Herrmann, W.A.; Kühn, F.E. Platinum Catalysis Revisited—Unraveling Principles of Catalytic Olefin Hydrosilylation. *ACS Catal.* **2016**, *6*, 1274–1284. [\[CrossRef\]](#)
- Zhou, Y.; Xu, X.; Sun, H.; Tao, G.; Chang, X.-Y.; Xing, X.; Chen, B.; Xu, C. Development of Highly Efficient Platinum Catalysts for Hydroalkoxylation and Hydroamination of Unactivated Alkenes. *Nat. Commun.* **2021**, *12*, 1953. [\[CrossRef\]](#) [\[PubMed\]](#)
- Wang, X.; Du, P.; Cheng, K.; Hua, X.; Xie, M.; Li, Y.; Zheng, Y.; Wang, Y.; Pi, C.; Zhang, S. Structural Regulation of Advanced Platinum-Based Core-Shell Catalysts for Fuel Cell Electrocatalysis. *Minerals* **2025**, *15*, 235. [\[CrossRef\]](#)
- Sahoo, D.; Deb, P.; Basu, T.; Bardhan, S.; Patra, S.; Sukul, P.K. Advancements in Platinum-Based Anticancer Drug Development: A Comprehensive Review of Strategies, Discoveries, and Future Perspectives. *Bioorg. Med. Chem.* **2024**, *112*, 117894. [\[CrossRef\]](#) [\[PubMed\]](#)
- Jin, S.; Guo, Y.; Wang, X. Development of Platinum Complexes for Tumor Chemoimmunotherapy. *Chem.—Eur. J.* **2024**, *30*, e202302948. [\[CrossRef\]](#)
- Clarke, M.L. Recent Advances in Homogeneous Catalysis Using Platinum Complexes. *Polyhedron* **2001**, *20*, 151–164. [\[CrossRef\]](#)
- Rebo, H.P.; Blekkan, E.A.; Bednářová, L.; Holmen, A. Deactivation of Pt-Sn Catalyst in Propane Dehydrogenation. *Stud. Surf. Sci. Catal.* **1999**, *126*, 333–340. [\[CrossRef\]](#)
- Bariás, O.A.; Holmen, A.; Blekkan, E.A. Propane Dehydrogenation over Supported Pt and Pt-Sn Catalysts: Catalyst Preparation, Characterization, and Activity Measurements. *J. Catal.* **1996**, *158*, 1–12. [\[CrossRef\]](#)
- Pregosin, P.S.; Rüegger, H. ^{119}Sn and ^{195}Pt NMR Spectroscopy of SnCl_3^- Complexes of Platinum and Palladium. Some Chemistry of the Complexes $(\text{Ph}_4\text{P})_2[\text{PtCl}_4]$ and $[\text{Pt}(\mu\text{-Cl})\text{Cl}(\text{PEt}_3)_2]$ with SnCl_2 . *Inorg. Chim. Acta* **1984**, *86*, 55–60. [\[CrossRef\]](#)
- Yasumori, I.; Hirabayashi, K. Homogeneous Catalysis by Pt(II)–Sn(II) Chloride Complex. Part 1.—Kinetics and Mechanisms of the Hydrogenations of Acetylene and Ethylene. *Trans. Faraday Soc.* **1971**, *67*, 3283–3296. [\[CrossRef\]](#)
- Dias, R.P.; Rocha, W.R. DFT Study of the Homogeneous Hydroformylation of Propene Promoted by a Heterobimetallic Pt–Sn Catalyst. *Organometallics* **2011**, *30*, 4257–4268. [\[CrossRef\]](#)
- Zhang, F.; Chen, K.; Jiang, Q.; He, S.; Chen, Q.; Liu, Z.; Kang, J.; Zhang, Q.; Wang, Y. Selective Transformation of Methanol to Ethanol in the Presence of Syngas over Composite Catalysts. *ACS Catal.* **2022**, *12*, 8451–8461. [\[CrossRef\]](#)
- Fricke, C.H.; Bamidele, O.H.; Bello, M.; Chowdhury, J.; Terejanu, G.; Heyden, A. Modeling the Effect of Surface Platinum–Tin Alloys on Propane Dehydrogenation on Platinum–Tin Catalysts. *ACS Catal.* **2023**, *13*, 10627–10640. [\[CrossRef\]](#)
- Rocha, W.R. Hydrogen Activation and Aldehyde Elimination Promoted by Homogeneous Pt–Sn Catalyst: A Theoretical Study. *J. Mol. Struct. THEOCHEM* **2004**, *677*, 133–143. [\[CrossRef\]](#)
- Johnston, V.J.; Chen, L.; Kimmich, B.F.; Chapman, J.T.; Zink, J.H. Direct and Selective Production of Ethanol from Acetic Acid Utilizing a Platinum/Tin Catalyst. U.S. Patent 2011/0263911A1, 27 October 2011.
- Young, J.F.; Gillard, R.D.; Wilkinson, G. 992. Complexes of Ruthenium, Rhodium, Iridium, and Platinum with Tin(II) Chloride. *J. Chem. Soc.* **1964**, 5176. [\[CrossRef\]](#)
- Cramer, R.D.; Lindsey, R.V.; Prewitt, C.T.; Stolberg, U.G. Five-Coordinate Platinum(II) Complexes. *J. Am. Chem. Soc.* **1965**, *87*, 658. [\[CrossRef\]](#)
- Nelson, J.H.; Alcock, N.W. Crystal and Solution Structure of Triphenylmethylphosphonium Pentakis(Trichlorostannyl)Platinate(II), $[\text{Ph}_3\text{PCH}_3]_3[\text{Pt}(\text{SnCl}_3)_5]$. *Inorg. Chem.* **1982**, *21*, 1196–1200. [\[CrossRef\]](#)
- Still, B.M.; Kumar, P.G.A.; Aldrich-Wright, J.R.; Price, W.S. ^{195}Pt NMR-Theory and Application. *Chem. Soc. Rev.* **2007**, *36*, 665–686. [\[CrossRef\]](#)
- Pregosin, P.S. Platinum NMR Spectroscopy. *Annu. Reports NMR Spectrosc.* **1986**, *17*, 285–349. [\[CrossRef\]](#)
- Momeni, B.Z.; Baleh, L.J.; Hamzeh, S.; Rominger, F. Insertion of SnCl_2 into Pt–Cl Bonds: Synthesis and Characterization of Four- and Five-Coordinate Trichlorostannylplatinum(II) Complexes. *J. Coord. Chem.* **2007**, *60*, 285–293. [\[CrossRef\]](#)

24. Priqueler, J.R.L.; Butler, I.S.; Rochon, F.D. An Overview of ^{195}Pt Nuclear Magnetic Resonance Spectroscopy. *Appl. Spectrosc. Rev.* **2006**, *41*, 185–226. [\[CrossRef\]](#)
25. Gilbert, T.M.; Ziegler, T. Prediction of ^{195}Pt NMR Chemical Shifts by Density Functional Theory Computations: The Importance of Magnetic Coupling and Relativistic Effects in Explaining Trends. *J. Phys. Chem. A* **1999**, *103*, 7535–7543. [\[CrossRef\]](#)
26. Koch, K.R.; Burger, M.R.; Kramer, J.; Westra, A.N. ^{195}Pt NMR and DFT Computational Methods as Tools towards the Understanding of Speciation and Hydration/Solvation of $[\text{PtX}_6]^{2-}$ ($\text{X} = \text{Cl}^-$, Br^-) Anions in Solution. *Dalton Trans.* **2006**, 3277–3284. [\[CrossRef\]](#)
27. Sterzel, M.; Autschbach, J. Toward an Accurate Determination of ^{195}Pt Chemical Shifts by Density Functional Computations: The Importance of Unspecific Solvent Effects and the Dependence of Pt Magnetic Shielding Constants on Structural Parameters. *Inorg. Chem.* **2006**, *45*, 3316–3324. [\[CrossRef\]](#)
28. Truflandier, L.A.; Autschbach, J. Probing the Solvent Shell with ^{195}Pt Chemical Shifts: Density Functional Theory Molecular Dynamics Study of PtII and PtIV Anionic Complexes in Aqueous Solution. *J. Am. Chem. Soc.* **2010**, *132*, 3472–3483. [\[CrossRef\]](#)
29. Autschbach, J.; Le Guennic, B. Solvent Effects on ^{195}Pt and ^{205}Tl NMR Chemical Shifts of the Complexes $[(\text{NC})_5\text{Pt-Tl}(\text{CN})_n]^{n-}$ ($n=0-3$), and $[(\text{NC})_5\text{Pt-Tl-Pt}(\text{CN})_5]^{3-}$ Studied by Relativistic Density Functional Theory. *Chem.—Eur. J.* **2004**, *10*, 2581–2589. [\[CrossRef\]](#) [\[PubMed\]](#)
30. Truflandier, L.A.; Sutter, K.; Autschbach, J. Solvent Effects and Dynamic Averaging of ^{195}Pt NMR Shielding in Cisplatin Derivatives. *Inorg. Chem.* **2011**, *50*, 1723–1732. [\[CrossRef\]](#) [\[PubMed\]](#)
31. Gabano, E.; Marengo, E.; Bobba, M.; Robotti, E.; Cassino, C.; Botta, M.; Osella, D. ^{195}Pt NMR Spectroscopy: A Chemometric Approach. *Coord. Chem. Rev.* **2006**, *250*, 2158–2174. [\[CrossRef\]](#)
32. Ondar, E.E.; Polynski, M.V.; Ananikov, V.P. Predicting ^{195}Pt NMR Chemical Shifts in Water-Soluble Inorganic/Organometallic Complexes with a Fast and Simple Protocol Combining Semiempirical Modeling and Machine Learning. *ChemPhysChem* **2023**, *24*, e202200940. [\[CrossRef\]](#)
33. Meßler, A.; Bahmann, H. Uncertainty-Aware Prediction of ^{195}Pt Chemical Shifts from Limited Data. *J. Chem. Inf. Model.* **2026**, *66*, 1498–1510. [\[CrossRef\]](#)
34. Semenov, V.A.; Samultsev, D.O.; Rusakova, I.L.; Krivdin, L.B. Computational Multinuclear NMR of Platinum Complexes: A Relativistic Four-Component Study. *J. Phys. Chem. A* **2019**, *123*, 4908–4920. [\[CrossRef\]](#)
35. Semenov, V.A.; Rusakov, Y.Y.; Samultsev, D.O.; Krivdin, L.B. Geometries and NMR Properties of Cisplatin and Transplatin Revisited at the Four-Component Relativistic Level. *Mendeleev Commun.* **2019**, *29*, 315–317. [\[CrossRef\]](#)
36. Tshipis, A.C.; Karapetsas, I.N. Accurate Prediction of ^{195}Pt NMR Chemical Shifts for a Series of Pt(II) and Pt(IV) Antitumor Agents by a Non-Relativistic DFT Computational Protocol. *Dalton Trans.* **2014**, *43*, 5409–5426. [\[CrossRef\]](#)
37. Tshipis, A.C.; Karapetsas, I.N. Accurate Prediction of ^{195}Pt -NMR Chemical Shifts for Hydrolysis Products of $[\text{PtCl}_6]^{2-}$ in Acidic and Alkaline Aqueous Solutions by Non-Relativistic DFT Computational Protocols. *J. Coord. Chem.* **2015**, *68*, 3788–3804. [\[CrossRef\]](#)
38. Tshipis, A.C.; Karapetsas, I.N. Prediction of ^{195}Pt NMR Chemical Shifts of Dissolution Products of $\text{H}_2[\text{Pt}(\text{OH})_6]$ in Nitric Acid Solutions by DFT Methods: How Important Are the Counterion Effects? *Magn. Reson. Chem.* **2016**, *54*, 656–664. [\[CrossRef\]](#) [\[PubMed\]](#)
39. Tshipis, A.C.; Karapetsas, I.N. Prediction of ^{195}Pt NMR of Photoactivable Diazido-and Azine-Pt(IV) Anticancer Agents by DFT Computational Protocols. *Magn. Reson. Chem.* **2017**, *55*, 145–153. [\[CrossRef\]](#) [\[PubMed\]](#)
40. Paschoal, D.; Fonseca Guerra, C.; de Oliveira, M.A.L.; Ramalho, T.C.; Dos Santos, H.F. Predicting Pt-195 NMR Chemical Shift Using New Relativistic All-Electron Basis Set. *J. Comput. Chem.* **2016**, *37*, 2360–2373. [\[CrossRef\]](#)
41. Kondrashova, S.A.; Latypov, S.K. Reliable DFT Protocol for Calculation of ^{195}Pt NMR Chemical Shifts. *Russ. Chem. Bull.* **2025**, *74*, 2970–2979. [\[CrossRef\]](#)
42. Carr, S.; Colton, R.; Dakternieks, D. Phosphorus-31, Tin-119 and Platinum-195 NMR Studies on Some Platinum(II)-Tin Bonded Compounds. *J. Organomet. Chem.* **1983**, *249*, 327–334. [\[CrossRef\]](#)
43. Starzewski, K.A.O.; Pregosin, P.S. ^{195}Pt -NMR Spectroscopy of Catalytically Active Complexes. Extremely Large Spin-Spin Coupling between Platinum and Tin. *Angew. Chem. Int. Ed. Engl.* **1980**, *19*, 316–317. [\[CrossRef\]](#)
44. Pregosin, P.S. The Multinuclear NMR Approach. Contributions to the Chemistry of Platinum. *Chimia* **1981**, *35*, 43. [\[CrossRef\]](#)
45. Pregosin, P.S.; Sze, S.N. The Reaction of SnCl_2 with the Complexes $\text{cis-PtCl}_2(\text{Phosphorus Ligand})_2$ as Studied by ^{31}P and ^{195}Pt NMR. *Helv. Chim. Acta* **1978**, *61*, 1848–1855. [\[CrossRef\]](#)
46. Starzewski, K.H.A.O.; Pregosin, P.S.; Rügger, H. ^{31}P -, ^{119}Sn - and ^{195}Pt -NMR. Studies of Trichlorostannate Complexes of Pt(II) and Pd(II). $^2J(^{119}\text{Sn}, ^{117}\text{Sn})$ -Values. *Helv. Chim. Acta* **1982**, *65*, 785–797. [\[CrossRef\]](#)
47. Albinati, A.; Pregosin, P.S.; Rügger, H. Trichlorostannate Complexes of Platinum. Synthesis, Multinuclear NMR Spectroscopy and x-Ray Crystallography of $\text{trans-}[\text{Pt}(\text{SnCl}_3)_2\text{P}(\text{OPh})_3]_2$ and Related Complexes. *Inorg. Chem.* **1984**, *23*, 3223–3229. [\[CrossRef\]](#)
48. Holt, M.S.; MacDougall, J.J.; Mathey, F.; Nelson, J.H. A Multinuclear NMR Investigation of Stannous Chloride Promoted Ligand Exchange of Platinum Phosphole Complexes. *Inorg. Chem.* **1984**, *23*, 449–453. [\[CrossRef\]](#)

49. Goodfellow, R.J.; Herbert, I.R. An NMR Study of the Insertion of Tin(II) Halides into a Platinum-Platinum Bond. *Inorg. Chim. Acta* **1982**, *65*, L161–L162. [\[CrossRef\]](#)
50. Albinati, A.; Von Gunten, U.; Pregosin, P.S.; Rugg, H.J. ^{195}Pt , ^{119}Sn and ^{31}P NMR Studies of Alkyl, Aryl and Acyl Trichlorostannate Complexes of Platinum(II). The Crystal Structure of *trans*-[Pt(SnCl₃)(COC₆H₅)(PEt₃)₂]. *J. Organomet. Chem.* **1985**, *295*, 239–256. [\[CrossRef\]](#)
51. Lee, C.; Yang, W.; Parr, R.G. Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron Density. *Phys. Rev. B* **1988**, *37*, 785–789. [\[CrossRef\]](#) [\[PubMed\]](#)
52. Stephens, P.J.; Devlin, F.J.; Chabalowski, C.F.; Frisch, M.J. Ab Initio Calculation of Vibrational Absorption and Circular Dichroism Spectra Using Density Functional Force Fields. *J. Phys. Chem.* **1994**, *98*, 11623–11627. [\[CrossRef\]](#)
53. Becke, A.D. Density-functional Thermochemistry. III. The Role of Exact Exchange. *J. Chem. Phys.* **1993**, *98*, 5648–5652. [\[CrossRef\]](#)
54. Hay, P.J.; Wadt, W.R. Ab Initio Effective Core Potentials for Molecular Calculations. Potentials for K to Au Including the Outermost Core Orbitals. *J. Chem. Phys.* **1985**, *82*, 299–310. [\[CrossRef\]](#)
55. Metz, B.; Stoll, H.; Dolg, M. Small-Core Multiconfiguration-Dirac–Hartree–Fock-Adjusted Pseudopotentials for Post- d Main Group Elements: Application to PbH and PbO. *J. Chem. Phys.* **2000**, *113*, 2563–2569. [\[CrossRef\]](#)
56. Weigend, F.; Ahlrichs, R. Balanced Basis Sets of Split Valence, Triple Zeta Valence and Quadruple Zeta Valence Quality for H to Rn: Design and Assessment of Accuracy. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297. [\[CrossRef\]](#)
57. Scalmani, G.; Frisch, M.J. Continuous Surface Charge Polarizable Continuum Models of Solvation. I. General Formalism. *J. Chem. Phys.* **2010**, *132*, 114110. [\[CrossRef\]](#)
58. Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Petersson, G.A.; Nakatsuji, H.; et al. *Gaussian 16*; Revision C.01; Gaussian, Inc.: Wallingford, CT, USA, 2016.
59. Alcock, N.W.; Nelson, J.H. The [PtCl₂(SnCl₃)₂]²⁻ Ion: Crystal Structure of Two Salts. *J. Chem. Soc. Dalt. Trans.* **1982**, 2415–2418. [\[CrossRef\]](#)
60. London, F. Théorie Quantique Des Courants Interatomiques Dans Les Combinaisons Aromatiques. *J. Phys. Le Radium* **1937**, *8*, 397–409. [\[CrossRef\]](#)
61. McWeeny, R. Perturbation Theory for the Fock-Dirac Density Matrix. *Phys. Rev.* **1962**, *126*, 1028–1034. [\[CrossRef\]](#)
62. Ditchfield, R. Self-Consistent Perturbation Theory of Diamagnetism. *Mol. Phys.* **1974**, *27*, 789–807. [\[CrossRef\]](#)
63. Wolinski, K.; Hinton, J.F.; Pulay, P. Efficient Implementation of the Gauge-Independent Atomic Orbital Method for NMR Chemical Shift Calculations. *J. Am. Chem. Soc.* **1990**, *112*, 8251–8260. [\[CrossRef\]](#)
64. Cheeseman, J.R.; Trucks, G.W.; Keith, T.A.; Frisch, M.J. A Comparison of Models for Calculating Nuclear Magnetic Resonance Shielding Tensors. *J. Chem. Phys.* **1996**, *104*, 5497–5509. [\[CrossRef\]](#)
65. Perdew, J.P.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple [Phys. Rev. Lett. 77, 3865 (1996)]. *Phys. Rev. Lett.* **1997**, *78*, 1396. [\[CrossRef\]](#)
66. Perdew, J.P.; Burke, K.; Wang, Y. Generalized Gradient Approximation for the Exchange–Correlation Hole of a Many-Electron System. *Phys. Rev. B* **1996**, *54*, 16533–16539. [\[CrossRef\]](#)
67. Carvalho, J.; Paschoal, D.; Fonseca Guerra, C.; Dos Santos, H.F. Nonrelativistic Protocol for Calculating the $^1J(^{195}\text{Pt}-^{15}\text{N})$ Coupling Constant in Pt(II)-Complexes Using All-Electron Gaussian Basis-Set. *Chem. Phys. Lett.* **2020**, *745*, 137279. [\[CrossRef\]](#)
68. E Silva, J.H.C.; Dos Santos, H.F.; Paschoal, D.F.S. Predicting Pt-195 Nmr Chemical Shift and $^1J(^{195}\text{Pt}-^{31}\text{P})$ Coupling Constant for Pt(0) Complexes Using the NMR-DKH Basis Sets. *Magnetochemistry* **2021**, *7*, 148. [\[CrossRef\]](#)
69. Paschoal, D.F.S.; Dos Santos, H.F. Predicting the Structure and NMR Coupling Constant $^1J(^{129}\text{Xe}-^{19}\text{F})$ of XeF₆ Using Quantum Mechanics Methods. *Phys. Chem. Chem. Phys.* **2021**, *23*, 7240–7246. [\[CrossRef\]](#) [\[PubMed\]](#)
70. de Andrade, T.F.C.B.; Dos Santos, H.F.; Fonseca Guerra, C.; Paschoal, D.F.S. Computational Prediction of Tc-99 NMR Chemical Shifts in Technetium Complexes with Radiopharmaceutical Applications. *J. Phys. Chem. A* **2022**, *126*, 5434–5448. [\[CrossRef\]](#)
71. Gomes, M.G.R.; De Souza, A.L.F.; Dos Santos, H.F.; De Almeida, W.B.; Paschoal, D.F.S. Assessment of a Computational Protocol for Predicting Co-59 NMR Chemical Shift. *Magnetochemistry* **2023**, *9*, 172. [\[CrossRef\]](#)
72. Gomes, M.G.R.; de Souza, C.R.S.; Paschoal, D.F.d.S.; De Almeida, W.B. Predicting Ti-49 NMR Chemical Shift with New NMR-DKH Basis Set. *J. Comput. Chem.* **2025**, *46*, e70258. [\[CrossRef\]](#)

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