

**Short thesis for the degree of doctor of philosophy
(PhD)**

**Preparation of water-soluble tetrahydrosalene
complexes and some of their catalytic properties**

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List of abbreviations

ESR	Electron Spin Resonance
ESI-TOF-MS	electrospray ionization time-of-flight mass spectrometry
ICP-OES	inductively coupled plasma optical emission spectrometry
NMR	Nuclear Magnetic Resonance
TOF	turnover frequency (h^{-1})
SC-XRD	single-crystal X-ray diffraction
p<i>K</i>_a	deprotonation constants

I. Introduction and objectives

Environmental have become an increasing priority for our society. There is also a growing demand for the use of low-cost metal catalysts in modern industrial technologies. The development of new, efficient metal complex catalysts is crucial to produce industrially significant raw materials and to make processes simpler and more sustainable.

N2O2-type ligands play an important role in the development of modern coordination chemistry and in the production of new metal complex catalysts. They also have important applications in pharmaceutical chemistry. Their derivatives are also increasingly used in medicinal chemistry, as they have been reported to have anti-tumour and cytotoxic effects, and thus have potential for use in *in vitro* and *in vivo* studies. Due to their diversity and ease of modification, the catalytic application of their metal complexes is significant as they can be used in a variety of chemical processes.

To this end, I have aimed at the preparation of new water-soluble *N2O2* donor ligands (sulfosalane) and their palladium and cheaper transition metal complexes and their solution equilibrium studies. Sulfosalane ligands and their metal complexes are characterised by a wide variety of coordination chemistries, since the structure of the resulting complexes is significantly influenced by the quality of the metal ion. The results obtained were intended to be used in the development of homogeneous catalytic reactions and in the elucidation of the mechanism of the reactions carried out. The parallel study of complex formation and catalysis is important, since the preparation of new catalysts requires a complex approach.

Thus, the most important novelty of my work is the pH-potentiometric determination of the stability of metal complexes, the calculation of their distribution as a function of the pH of aqueous solutions, and their

comparison to the pH dependence of their catalytic activity - in short, the linking of coordination chemistry and homogeneous catalysis.

The aim of my PhD research was also to extend the study of complex formation and catalytic properties to cheaper metal ions besides palladium, in particular Ni(II) and Cu(II), and to apply the new complexes to catalyse synthetically important reactions (hydrogenation, C-C cross-coupling, Henry reaction) in aqueous media.

We aim at the solution equilibrium characterisation of the synthesised sulphonated salane ligands and their transition metal complexes. These studies can greatly facilitate the preparation of different transition metal complexes and the understanding of their catalytic properties, as well as the investigation of the mechanism of the individual reactions.

I want to determine the optimal application conditions of the prepared Pd(II), Ni(II) and Cu(II) sulphosalane catalysts in selected coupling reactions and hydrogenation reactions: to study the effect of different solvents and bases on the reactions, to compare the conversion values of experiments carried out at different pressures and temperatures.

In the processing of catalytic reactions, including product analysis, the use of organic solvents is often unavoidable. *However, in line with the principles of green chemistry, we need to minimise the impact on the environment by replacing the use of toxic organic solvents. This is why our aim was to develop a method for the production and purification of biaryl derivatives with excellent yields in the Suzuki-Miyaura coupling process without the use of organic solvents.*

One of the pillars of sustainable development is the environmentally friendly treatment of used catalysts: reuse or recycling. There is also an economic dimension to the maximisation of the recovery and reuse of expensive precious-metal based catalysts. *A further aim of my research was therefore to investigate the reuse of new palladium complexes in several successive reactions.*

II. Experimental methods

^1H - and ^{13}C -NMR spectroscopy, ESI-TOF-MS mass spectrometry, infrared spectroscopy and elemental analysis were used to characterise the ligands and their Pd(II) complexes.

For the characterization of paramagnetic Cu(II) complexes, we had the opportunity to perform ESR spectroscopy measurements in the framework of national and international collaborations.

The molecular structure of the synthesized sulfonated salane ligands and some of their metal complexes was also confirmed by single crystal X-ray diffraction (SC-XRD) measurements.

For the different sulphonated tetrahydrosalene ligands and their metal complexes, these measurements were further complemented by pH-potentiometric titrations. This method was used not only to investigate complex formation but also to check the purity of the ligands.

The deprotonation constants of the ligands were determined, as well as the composition and stability constants of the metal complexes formed (Pd(II), Cu(II), Ni(II) complexes). NMR-pH titrations were also performed to determine the micro- and macro-constants of the ligands. Solutions of copper(II) and nickel(II) complexes were analysed by UV and UV-visible spectrophotometry.

The Suzuki-Miyaura reactions were performed using the Schlenk technique and the hydrogenation reactions were carried out in a specially designed pressurized glass reactor.

The purity of the biphenyls produced by Suzuki-Miyaura coupling was also checked by gas chromatography and ^1H - and ^{13}C -NMR spectroscopy. The palladium content of the C-C coupled products from the Suzuki-Miyaura reaction was determined by ICP-OES. The analysis of the products in the hydrogenation reactions was determined by gas chromatography. For the nitroaldol (Henry) reactions, I used ^1H -NMR spectroscopy to determine the conversion.

III. New scientific results

I did my PhD research in the field of aqueous organometallic catalysis with two main objectives. *First, I wished to substantially increase the family of water-soluble and water-stable derivatives of salen-type ligands, namely the sulfosalans, and our knowledge on their metal complex forming properties. Second, I planned the use of Pd(II)-, Ni(II)-, and Cu(II)-complexes –obtained with the use of these new ligands– as catalysts for synthetically useful reactions.* Throughout my work I strived for the application of the data determined for complex formation and stability in the choice and optimization of reaction conditions, as well as the use of structural features of the metal complex catalysts in the evaluation and discussion of the results on catalysis. In fact, these approaches are the ones which connect the two major research objectives.

1. Synthesis and characterization of new sulfonated salen-type ligands

1.1 Altogether 12 sulfonated salen ligands were synthesized and characterized with the use of ^1H - and ^{13}C -NMR, IR, ESI-MS, SC-XRD, ESR methods. diffractometry, too (**Figure 1**).

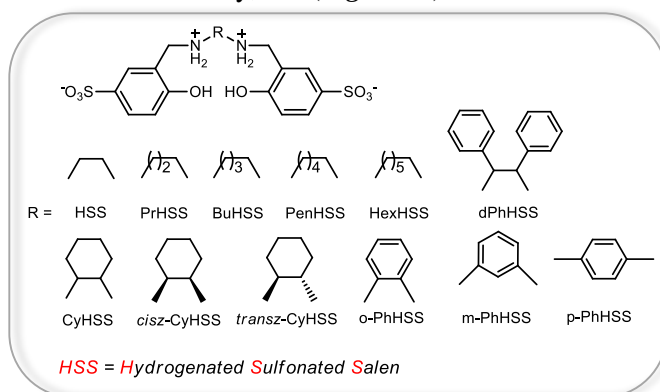


Figure 1. The formulae of the investigated ligands

Of these, 5 have not been described in the literature earlier, the other 7 were prepared for purposes of comparison. The molecular structures of 7 sulfosalan ligands were determined by single crystal X-ray.

2. Synthesis and characterization of Pd(II)-, Ni(II)-, and Cu(II)-complexes containing sulfonated salan-type ligands

2.1 The same complexes could be obtained in a mechanochemical procedure, too, which involved the thorough grinding of the sulfosalan ligand, $\text{Na}_2[\text{PdCl}_4]$ and NaHCO_3 in an agate mortar.

Altogether, eight Pd(II)-sulfosalan complexes were synthesized in the reaction of $(\text{NH}_4)_2[\text{PdCl}_4]$ with the appropriate ligand in slightly basic aqueous solutions; the products were isolated by precipitation with cold ethanol, characterized by yields usually around 80-90 %.

In my work, I succeeded in growing single crystals suitable for X-ray diffraction measurements from three new Pd(II) complexes ($\text{Na}_2[\text{Pd}(\text{PrHSS})]$; $\text{Na}_2[\text{Pd}(\text{BuHSS})]$; $\text{Na}_2[\text{Pd}(\text{dPhHSS})]$) (**Figure 2**). These are the first sulfonated salane-containing Pd(II) complexes in the literature. Their study is an excellent complement to the spectroscopic characterization of the complexes.

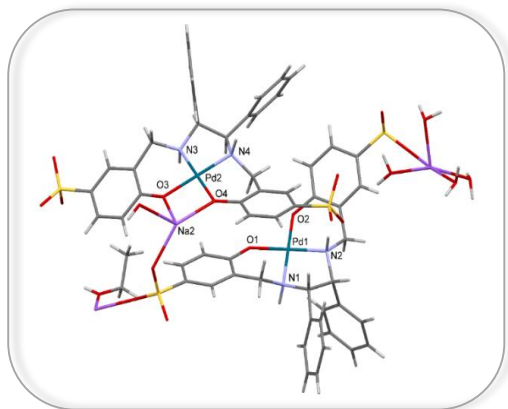


Figure 2. Molecular structure of the $\text{Na}_2[\text{Pd}(\text{dPhHSS})]$ complex

2.2 $K_2[Ni(HSS)]$, $K_2[Ni(CyHSS)]$, and $K_2[Ni(dPhHSS)]$ were prepared in methanol, in the reaction of the sulfosalan ligand and $Ni(CH_3COO)_2$ (yields 83-90 %).

2.3 In reactions of $Cu(CH_3COO)_2$ with the appropriate ligand in slightly basic aqueous solutions, altogether five Cu(II)-sulfosalan complexes were obtained; these were isolated by precipitation with ethanol (yields: 59-92 %).

In general, structural characterization of the complexes was achieved with the use of 1H - and ^{13}C -NMR, IR, and ESI-MS measurements. In the case of the Cu(II)-complexes, detailed ESR and UV-Vis spectroscopic studies were also carried out, furthermore, the solid state structures of one complexes have been determined with SC-XRD, too.

2.4 For all the complexes, the structural investigations revealed tetradentate *O,N,N,O* coordination of the sulfosalan ligand in a distorted square planar geometry; the extent of distortion depended on the size and structure of the bridge connecting the nitrogen atoms of the diamine unit (diamine bridge).

3. Protonation equilibria of sulfonated salan-type ligands in aqueous solution

3.1 Deprotonation of the HSS, PrHSS, BuHSS, *cis*-CyHSS, *trans*-CyHSS, and dPhHSS sulfosalans were studied by pH-potentiometric titrations (**Table 1**). In the potentiometrically measurable pH-region, altogether four deprotonation constants (pK_a) could be determined, belonging to the deprotonation of the two phenolic and the two (protonated) secondary amino groups.

Table 1. Stepwise Deprotonation Constants (pK_a) of the Ligands $(I = 0.2 \text{ M KCl}, T = 298 \text{ K})$

	<i>HSS</i>	<i>PrHSS</i>	<i>BuHSS</i>	<i>cis-</i> <i>CyHSS</i>	<i>trans-</i> <i>CyHSS</i>	<i>dPhHSS</i>
H ₄ L	6,00(8)	6,93(8)	6,94(4)	4,32(5)	4,45(4)	6,13(6)
H ₃ L	7,44(7)	7,82(8)	7,81(4)	7,71(4)	7,65(4)	6,68(7)
H ₂ L	8,75(6)	9,57(7)	10,08(3)	9,10(4)	9,13(4)	9,33(6)
HL	10,64(4)	11,28(4)	11,47(2)	11,42(2)	11,37(2)	9,86(6)
ΣH ₄ L	32,83	35,60	36,30	32,55	32,60	32,00

^a 3σ standard deviations are in parentheses.

3.2 It follows unambiguously from the pH-dependent ¹H- and ¹³C-NMR spectra that the smallest measurable pK_a belongs to the deprotonation of one of the secondary ammonium ions, resulting in formation of an intramolecular hydrogen bridge between the amino and the protonated phenolic-OH groups. Further increase of the pH results first in deprotonation of the phenolic hydroxyls, while the highest pK_a (e.g. $pK_a(\text{HL}) = 10.64$ for HSS) belongs to the deprotonation of the other amino group.

4. Formation of sulfosalan-ligated Pd(II)-, Ni(II)-, and Cu(II)-complexes in aqueous solutions

4.1 Stability constants of Pd(II) and Ni(II) sulfosalan complexes were determined potentiometrically with the use of HSS, PrHSS, and BuHSS ligands, additionally, *cis*-CyHSS, *trans*-CyHSS, and dPhHSS were also studied in the case of Cu(II)-complexes.

4.2 In all systems, it was established that sulfosalan ligands were excellent complex-forming agents for the mentioned metal ions, capable for preventing formation of hydroxo-complexes even in basic solutions. With all three metal ions, formation of *O,N,N,O* coupled-chelates were

observed, and the resulting complexes showed axially distorted square planar geometries. These conclusions were supported both by UV-Visible spectroscopic measurements (for Ni(II) and Cu(II) complexes) and by the ESR spectroscopic data (for Cu(II) complexes).

4.3 Complexation starts with the formation of $[\text{Pd}(\text{HL})\text{Cl}]$, $[\text{Ni}(\text{HL})]$, and $[\text{Cu}(\text{HL})]$ species, respectively (stability constants for all complexes were determined, except the Cu(II)/dPhHSS system), in overlap with formation of the $[\text{ML}]$ complex (**Figure 3**). The complex distribution curves (calculated with the use of the stability constants) revealed that in aqueous solutions of the studied Pd(II) and Ni(II) complexes at $\text{pH} \geq 8$, the dominant species have the $[\text{ML}]$ composition, which gives clues to the explanation of the pH dependence of catalytic reactions.

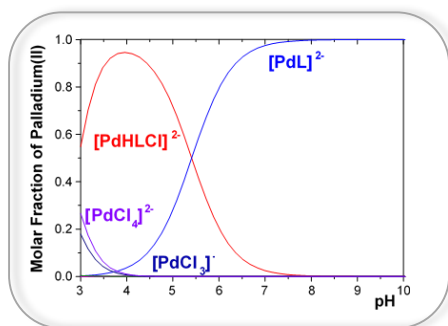


Figure 3. The distribution of the complexes formed in the Pd(II):HSS 1:1 system as a function of pH, ($c_L = 2.0 \text{ mM}$)

5. Application of Pd(II)-sulfosalan complexes in aqueous-phase Suzuki-Miyaura C-C cross-coupling reactions

5.1 All Pd(II)-sulfosalan complexes were found excellent catalysts in Suzuki-Miyaura C-C cross-coupling reactions. The new Pd(II)-complexes actively catalyzed the reaction of the most diverse aryl halides and phenylboronic acids.

5.2 The effect of the diamine bridge on the catalytic activity of Pd(II)-sulfosalan complexes was studied in detail. The highest catalytic activity was shown by $\text{Na}_2[\text{Pd}(\text{dPhHSS})]$ ($\text{TOF} = 23000 \text{ h}^{-1}$), while the lowest one was observed with $\text{Na}_2[\text{Pd}(\text{HSS})]$ ($\text{TOF} = 3250 \text{ h}^{-1}$).

5.3 With a wide array of measurements, conditions of the Suzuki-Miyaura C-C cross-coupling reactions were optimized for the maximum biphenyl yields (**Figure 4.**). It should be emphasized, that the practically water-insoluble biphenyl products could be isolated with simple filtration and purified with washing with dilute aqueous hydrochloric acid solution. Of the 20 biphenyl derivatives, synthesised with the use of the above process, palladium content of 14 products did not exceed 5 ppm, regarded acceptable in industrial synthesis of pharmaceutically active ingredients (API-s).

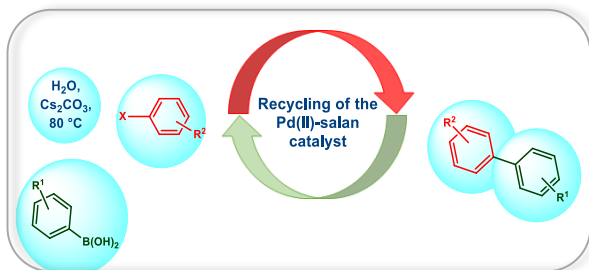


Figure 4. The catalysts, dissolved in the aqueous phase, could be used repeatedly

5.4 The catalysts, dissolved in the aqueous phase, could be used repeatedly (**Figure 4**). For example, the $\text{Na}_2[\text{Pd}(\text{BuHSS})]$ catalyst was applied for the synthesis of 4-acetylbiphenyl in three consecutive runs with no significant decrease of its catalytic activity.

6. Application of a Pd(II)- and Ni(II)-sulfosalan catalyst in aqueous-phase redox isomerization and hydrogenation reactions

6.1 The catalytic activity of $[\text{Pd}(\text{HSS})]$ was also determined as a function of the pH. Comparison of the pH-dependence of the catalytic activity to the species distribution determined by pH-potentiometry led to the conclusion that $[\text{PdL}]^{2-}$ possesses the highest catalytic activity in this reaction (**Figure 3**).

Although this approach may help in identifying actual catalytic species in homogeneous catalysis in aqueous solutions, nevertheless, the results should be evaluated with due care, especially when there is a considerable gap between the experimental conditions of speciation and catalytic studies (**Figure 5**).

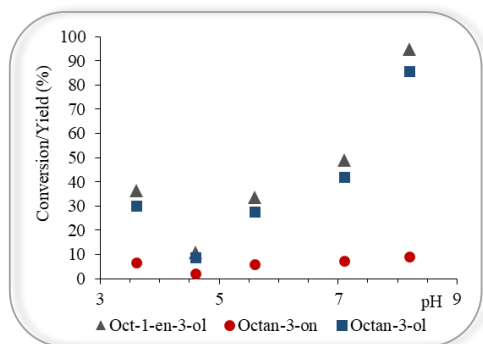


Figure 5. Conversion of oct-1-en-3-ol (\blacktriangle), yields of octan-3-ol (\blacksquare) and octan-3-one (\bullet) in hydrogenation and redox isomerization of oct-1-en-3-ol catalyzed by $\text{Na}_2[\text{Pd}(\text{HSS})]$ as a function of pH

Conditions: $2.5 \cdot 10^{-7}$ mol $\text{Na}_2[\text{Pd}(\text{HSS})]$; $2.5 \cdot 10^{-4}$ mol oct-1-en-3-ol; $V = 3$ ml acetate buffer; $I = 0.2$ M KCl; $p(\text{H}_2) = 1$ bar; $t = 30$ perc; $T = 40$ °C.

6.2 Of the newly synthesized Ni(II)-sulfosalan complexes, $K_2[Ni(HSS)]$ was studied as catalyst in redox isomerization of oct-1-en-3-ol in aqueous systems. The reaction took place only in the presence of H_2 , however, then the major product was the saturated alcohol, octan-3-ol (highest yield 90 %, depending on reaction conditions). The yield of the product of redox isomerization, octan-3-one, did not exceed 6 %. Similar selectivity was observed in the $K_2[Ni(HSS)]$ -catalyzed hydrogenation of estragol (4-allyl-anisole) in aqueous media under mild conditions.

The major product was the hydrogenated estragol, i.e. *p*-propyl-anisole, and the reaction mixtures contained only small mounts (2-5 %) of the isomerized derivatives, *trans*-, and *cis*-anethol. To the best of my knowledge, $K_2[Ni(HSS)]$ is the first Ni(II)-based, water-soluble and hydrolytically stable, sulfosalan-ligated complex catalyst capable for hydrogen activation and hydrogenation.

7. Application of Cu(II)-sulfosalan catalysts in aqueous-phase Henry-reactions

7.1 The nitroaldol reaction (Henry-reaction) of nitromethane and benzaldehyde and four other benzaldehyde derivatives was studied in water or in water-methanol mixtures, as solvents, with the use of four Cu(II)-sulfosalan complexes as catalysts. Of the studied complexes, the highest activity was shown by $Na_2[Cu(dPhHSS)]$, however, all the other complexes, too were superior to Cu(II)-acetate (**Figure 6**).

7.2 The pH-dependence of the reaction rate was determined in the case of the $Na_2[Cu(dPhHSS)]$ catalyst. Comparison of the pH-dependence of the reaction rate to the distribution of complex species (determined potentiometrically for the Cu(II)/dPhHSS system), it was unequivocally established, that the catalytic activity belongs to the $[CuL]$ Cu(II)-sulfosalan species and not to uncomplexed Cu^{2+} ions arising from dissociation of the sulfosalan complex.

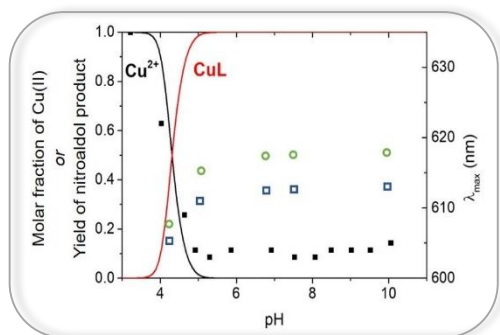


Figure 6. Distribution of the complexes formed in the Cu(II)/dPhHSS 1/1 systems and the λ_{max} values at the d-d band (■) obtained by UV-vis spectroscopy as a function of pH ($c_L = 2$ mM, $T = 298$ K). The open symbols (□ and ○) represent the yield of the nitroaldol product in the Henry reaction of benzaldehyde and nitromethane after 19 h and 36 h, respectively. Yields are expressed as mole fractions of the initial benzaldehyde amount (conditions of the catalytic reaction: 0.5 mmol benzaldehyde, 2.5 mmol nitromethane, 0.025 mmol $\text{Na}_2[\text{Cu}(\text{dPhHSS})]$, 2 mL water, 75 °C).

IV. Possible applications of the results

The results confirm, that sulfonated salans form stable complexes with several metal ions in aqueous solutions. Several of these complexes proved active catalysts in various aqueous-phase reactions, such as C-C cross-coupling, hydrogenation, and the Henry-reaction, and retained their stability also under the conditions of catalysis. Application of water as solvent allows simple isolation of water-insoluble reaction products and/or the repeated use of the catalyst dissolved in the aqueous phase.

On the basis of the results obtained so far, it seems worthwhile to extend the studies also for sulfosalan complexes of other metal ions, such as Ru(II), Ir(III), Co(II) or Mn(II) which play outstanding role in homogeneous catalysis, or just emerge as such recently.

V. Acknowledgements

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VI. List of publications related to the dissertation

Publications related to the dissertation

[1] **Szilvia Bunda**, Antal Udvardy, Krisztina Voronova, Ferenc Joó: **Organic Solvent-Free, Pd(II)-Salan Complex-Catalyzed Synthesis of Biaryls via Suzuki–Miyaura Cross-Coupling in Water and Air.**

J. Org. Chem. **2018**, 83, 15486–15492

DOI: 10.1021/acs.joc.8b02340

IF: 4.805, Q1

[2] Norbert Lihi, **Szilvia Bunda**, Antal Udvardy, Ferenc Joó: **Coordination chemistry and catalytic applications of Pd(II)-, and Ni(II)-sulfosalan complexes in aqueous media.**

J. Inorg. Biochem. **2020**, 203 1–7

DOI: 10.1016/j.jinorgbio.2019.110945

IF: 3.224, Q2

[3] **Szilvia Bunda**, Krisztina Voronova, Ágnes Kathó, Antal Udvardy, Ferenc Joó: **Palladium (II)-Salan Complexes as Catalysts for Suzuki–Miyaura C–C Cross-Coupling in Water and Air. Effect of the Various Bridging Units within the Diamine Moieties on the Catalytic Performance.**

Molecules, **2020**, 25, 3993.

DOI: 10.3390/molecules25173993

IF: 3.267, Q1

[4] **Szilvia Bunda**, Nóra Veronika May, Dóra Bonczidai-Kelemen, Antal Udvardy, H. Y. Vincent Ching, Kevin Nys, Mohammad Samanipour, Sabine Van Doorslaer, Ferenc Joó, Norbert Lihi: **Copper(II) Complexes of Sulfonated Salan Ligands: Thermodynamic and Spectroscopic Features and Applications for Catalysis of the Henry Reaction.**

Inorg. Chem. **2021**, 60, 11259–11272

DOI: 10.1021/acs.inorgchem.1c01264

IF: 5.165, Q1

List of other publications

[5] Réka Gombos, **Szilvia Bunda**, Brigitta Nagyházi, Ferenc Joó: **Homogeneous catalytic hydrogenation of lipids in aqueous dispersions and bacterial cell membranes with an efficient water-soluble Pd(II)-sulfosalan catalyst, Na₂[Pd(HSS)].**

Catal. Commun., **2020**, 147, 106153.

DOI:10.1016/j.catcom.2020.106153

IF: 3.612, Q1

[6] Mihály Purgel, Péter Pál Fehér, Álex Kálmán Balogh, **Szilvia Bunda**, Ferenc Joó: **Water-mediated formation of hydride derivates from flexible Pd-salan complexes: A DFT study.**

Mol. Catal., **2021**, 500, 111331.

DOI: 10.1016/j.mcat.2020.111331

IF: 3.387, Q1



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MTMT ID: 10066108

List of publications related to the dissertation

Foreign language scientific articles in international journals (4)

1. **Bunda, S.**, May, N. V., Bonczidai-Kelemen, D., Udvardy, A., Ching, H. Y. V., Nys, K., Samanipour, M., Van Doorslaer, S., Joó, F., Lihí, N.: Copper(II) Complexes of Sulfonated Salan Ligands: Thermodynamic and Spectroscopic Features and Applications for Catalysis of the Henry Reaction.
Inorg. Chem. 60 (15), 11259-11272, 2021. ISSN: 0020-1669.
DOI: <http://dx.doi.org/10.1021/acs.inorgchem.1c01264>
IF: 5.165 (2020)
2. Lihí, N., **Bunda, S.**, Udvardy, A., Joó, F.: Coordination chemistry and catalytic applications of Pd(II)-, and Ni(II)-sulfosalan complexes in aqueous media.
J. Inorg. Biochem. 203, 1-7, 2020. ISSN: 0162-0134.
DOI: <http://dx.doi.org/10.1016/j.jinorgbio.2019.110945>
IF: 4.155
3. **Bunda, S.**, Voronova, K., Kathó, Á., Udvardy, A., Joó, F.: Palladium (II)-Salan Complexes as Catalysts for Suzuki-Miyaura C-C Cross-Coupling in Water and Air. Effect of the Various Bridging Units within the Diamine Moieties on the Catalytic Performance.
Molecules. 25, 1-21, 2020. EISSN: 1420-3049.
DOI: <https://doi.org/10.3390/molecules25173993>
IF: 4.411
4. **Bunda, S.**, Udvardy, A., Voronova, K., Joó, F.: Organic Solvent-Free, Pd(II)-Salan Complex-Catalyzed Synthesis of Biaryls via Suzuki-Miyaura Cross-Coupling in Water and Air.
J. Org. Chem. 83 (24), 15486-15492, 2018. ISSN: 0022-3263.
DOI: <https://doi.org/10.1021/acs.joc.8b02340>
IF: 4.745





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List of other publications

Foreign language scientific articles in international journals (2)

5. Purgel, M., Fehér, P. P., Balogh, Á. K., **Bunda, S.**, Joó, F.: Water-mediated formation of hydride derivatives from flexible Pd-salan complexes: A DFT study.

Molecular Catalysis. 500, 1-9, 2021. ISSN: 2468-8231.

DOI: <https://doi.org/10.1016/j.mcat.2020.111331>

IF: 5.062 (2020)

6. Gombos, R., **Bunda, S.**, Nagyházi, B., Joó, F.: Homogeneous catalytic hydrogenation of lipids in aqueous dispersions and bacterial cell membranes with an efficient water-soluble Pd(II)-sulfosalan catalyst, Na₂[Pd(HSS)].

Catal. Commun. 147, 1-5, 2020. ISSN: 1566-7367.

DOI: <https://doi.org/10.1016/j.catcom.2020.106153>

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Total IF of journals (publications related to the dissertation): 18,476

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