Full list of publication in the 2015-2025 period[1-59]

Jean-Pierre Djukic

1. Hamdaoui, M., et al., *Quantum Hydrogen Tunneling in an Iridium Dihydride Complex.* J. Am. Chem. Soc., 2025. **147**(27): p. 23458–23472. 10.1021/jacs.4c17482.
2. Groslambert, L., et al., *Chalcogen Bonding with Telluronium Cations: toward Selective Population of Tellurium σ-Holes by Lewis Bases.* J Org Chem, 2025. **90**(24): p. 8254-8268. 10.1021/acs.joc.5c00744.
3. Li, Y., et al., *Cis-Chelating Diphosphanes for Intracavity Nickel(II)-Catalyzed Ethylene Oligomerization.* Chem. Eur. J., 2025. **31**(34): p. e202501188. 10.1002/chem.202501188.
4. Louaileche, T., et al., *SC-XRD investigation, DFT/TD-DFT, XRD/HSA-interaction, imine↔enol tautomerization and catecholase potential of new Zwitterionic pyran-2-one Schiff base ligand.* J. Indian Chem. Soc., 2025. **102**(8): p. 101842. 10.1016/j.jics.2025.101842.
5. Antuna-Horlein, C. and J.-P. Djukic, *Unlocking Catalysis Using Oxidatively Induced Reductive Elimination.* Chem. Eur. J., 2025. **31**(18): p. e202404341. 10.1002/chem.202404341.
6. Groslambert, L., et al., *Affinity of Telluronium Chalcogen Bond Donors for Lewis Bases in Solution: A Critical Experimental-Theoretical Joint Study.* Chem. Eur. J., 2024. **30**(7): p. e202302933. 10.1002/chem.202302933.
7. Wang, Z., Y. Cornaton, and J.-P. Djukic, *Triplet State-Promoted Kumada-Corriu Coupling Catalyzed by Hydrotris(3,5-diisopropylpyrazolyl)boratocobalt(III)diiodide.* Eur. J. Inorg. Chem., 2024. **27**(34): p. e202400420. 10.1002/ejic.202400420.
8. Chetioui, S., et al., *Synthesis and characterizations of a novel trans-Pd(O,N)2 complex with an AZO-dye ligand: Crystal structure, theoretical studies and DNA binding interactions.* Sci. Afr., 2024. **26**: p. e02411. 10.1016/j.sciaf.2024.e02411.
9. Eliwa, E.M., A.H. Bedair, and J.-P. Djukic, *Transition metal-catalyzed C(sp^2/sp^3)-H α-fluoroalkenylation from gem-(bromo/di)fluoroalkenes to monofluoroalkenes: scope, mechanisms, and synthetic applications.* Org. Biomol. Chem., 2024. **22**(34): p. 6860-6904. 10.1039/d4ob01044b.
10. Khadraoui, H., et al., *Joint Experimental/Theoretical Investigation of the Chemoselective Iridium(III) Metallacycle-Catalyzed Reduction of Substituted γ-Lactams by Et3SiH.* Organometallics, 2024. **43**(24): p. 3106-3122. 10.1021/acs.organomet.4c00044.
11. Ali, M., et al., *Follow-Up Study of Trans-C to Cis-C Thermally or Photochemically Induced Isomerization of Terpyridine Adducts of Cycloruthenated 2-Aryl-2'-pyridine Compounds.* Inorg. Chem., 2024. **63**(11): p. 4867-4874. 10.1021/acs.inorgchem.3c03671.
12. Behzadi, M., et al., *Electrophilic Si-H Activation by Acetonitrilo Benzo[h]quinoline Iridacycles: Influence of Electronic Effects in Catalysis.* Chem. - Eur. J., 2023. **29**(43): p. e202300811. 10.1002/chem.202300811.
13. Loir-Mongazon, L., et al., *Activation Barriers for Cobalt(IV)-Centered Reductive Elimination Correlate with Quantified Interatomic Noncovalent Interactions.* Synlett, 2023. **34**(10): p. 1169-1173. 10.1055/a-1937-9296.
14. Baumgarten, G., et al., *Assessment of the impact of static field inhomogeneity on the performance of miniaturized nmr devices.* IEEE Trans. Magn., 2023. **59**(2): p. 6100306. 10.1109/tmag.2022.3215674.

15. Antuna-Horlein, C., et al., *Cobalt Nanoparticles Formed upon Reaction of Cp*Co(III) Metallacycles with Na[BHEt3] Show Catalytic Activity in the Hydrosilylation of Aryl Ketones, Aldehydes and Nitriles.* Eur. J. Inorg. Chem., 2023. **26**(6): p. e202200563. 10.1002/ejic.202200563.
16. Mili, A., et al., *Tautomerization of diazene<=>hydrazine via single proton tautomerization, spectral, XRD/HSA-interactions, optical and DFT/TD-DFT of new hydrazine ligand.* J. Mol. Struct., 2023. **1272**: p. 134113. 10.1016/j.molstruc.2022.134113.
17. Hamdaoui, M., et al., *An Iridium-Stabilized Borenium Intermediate.* J. Am. Chem. Soc., 2022. **144**(40): p. 18359-18374. 10.1021/jacs.2c06298.
18. Weiss, R., et al., *Deciphering the Role of Noncovalent Interactions in the Conformations of Dibenzo-1,5-dichalcogenocines.* ChemPlusChem, 2022. **87**(4): p. e202100518. 10.1002/cplu.202100518.
19. Milovanovic, M.R., et al., *The Thermochemistry of Alkyne Insertion into a Palladacycle Outlines the Solvation Conundrum in DFT.* Eur. J. Inorg. Chem., 2021. **2021**(45): p. 4690-4699. 10.1002/ejic.202100750.
20. Cornaton, Y. and J.-P. Djukic, *Noncovalent Interactions in Organometallic Chemistry: From Cohesion to Reactivity, a New Chapter.* Acc. Chem. Res., 2021. **54**(20): p. 3828-3840. 10.1021/acs.accounts.1c00393.
21. Wu, F., et al., *Fate of Cobaltacycles in Cp*Co-Mediated C-H Bond Functionalization Catalysis: Cobaltacycles May Collapse upon Oxidation via Co(IV) Species.* Organometallics, 2021. **40**(15): p. 2624-2642. 10.1021/acs.organomet.1c00301.
22. Bougueria, H., et al., *Crystal structure and Hirshfeld surface analysis of 1-[(E)-2-(5-chloro-2-hydroxyphenyl)hydrazin-1-ylidene]naphthalen-2(1H)-one.* Acta Crystallogr., Sect. E: Crystallogr. Commun., 2021. **77**(6): p. 672-676. 10.1107/s2056989021005491.
23. Chouk, R., et al., *A combined DFT and experimental study into the optoelectronic and charge transport properties of ninhydrin-glycine Schiff base complexes for efficient LED applications.* Opt. Quantum Electron., 2021. **53**(4): p. 180. 10.1007/s11082-021-02816-z.
24. Chetioui, S., et al., *Cu(II) coordination polymer bearing diazenyl-benzoic ligand: Synthesis, physico-chemical and XRD/HSA-interactions.* J. Mol. Struct., 2021. **1229**: p. 129604. 10.1016/j.molstruc.2020.129604.
25. Chetioui, S., et al., *Synthesis, spectroscopic characterization, crystal structure and theoretical investigation of two azo-palladium (II) complexes derived from substituted (1-phenylazo)-2-naphtol.* Transition Met. Chem. (Dordrecht, Neth.), 2021. **46**(2): p. 91-101. 10.1007/s11243-020-00425-5.
26. Chouk, R., et al., *A computational and numerical studies of OLED based on ninhydrin-glycine Schiff base complex.* IEEE Trans. Electron Devices, 2020. **67**(12): p. 5581-5586. 10.1109/ted.2020.3031879.
27. Milovanovic, M.R., et al., *Joint Isotherm Calorimetric Titration-DFT Investigation of the Demethoxy-Amination of Fischer Carbenes.* J. Organomet. Chem., 2020. **929**: p. 121582. 10.1016/j.jorganchem.2020.121582.
28. Corre, Y., et al., *One-Pot Controlled Reduction of Conjugated Amides by Sequential Double Hydrosilylation Catalyzed by an Iridium(III) Metallacycle.* Eur. J. Org. Chem., 2020. **2020**(39): p. 6212-6220. 10.1002/ejoc.202001061.
29. Milovanovic, M.R., et al., *The Affinity of Some Lewis Bases for Hexafluoroisopropanol as a Reference Lewis Acid: An ITC/DFT Study.* ChemPhysChem, 2020. **21**(18): p. 2136-2142. 10.1002/cphc.202000560.
30. Wu, F., et al., *Making Base-Assisted C-H Bond Activation by Cp*Co(III) Effective: A Noncovalent Interaction-Inclusive Theoretical Insight and Experimental Validation.* Organometallics, 2020. **39**(14): p. 2609-2629. 10.1021/acs.organomet.0c00253.

31. Ulm, F., et al., *Hydroboration of Alkenes Catalysed by a Nickel N-Heterocyclic Carbene Complex: Reaction and Mechanistic Aspects.* Chem. - Eur. J., 2020. **26**(41): p. 8916-8925. 10.1002/chem.202000289.
32. Werle, C., et al., *μ-Carbonyl-bis(carbonyl{η^5-[tricarbonyl(η^6-2-methylindenyl)chromium(0)]rhodium(III)})(Rh-Rh).* IUCrData, 2019. **4**(5): p. x190573. 10.1107/s241431461900573x.
33. Jerhaoui, S., et al., *Asymmetric, Nearly Barrierless C(sp^3)-H Activation Promoted by Easily-Accessible N-Protected Aminosulfoxides as New Chiral Ligands.* ACS Catal., 2019. **9**(3): p. 2532-2542. 10.1021/acscatal.8b04946.
34. Hamdaoui, M. and J.-P. Djukic, *Noncovalent interactions in key metal-centred catalytic intermediates: structure-electronic relationship.* RSC Catal. Ser., 2019. **36**: p. 579-607.
35. Cornaton, Y. and J.-P. Djukic, *A noncovalent interaction insight onto the concerted metallation deprotonation mechanism.* Phys. Chem. Chem. Phys., 2019. **21**(36): p. 20486-20498. 10.1039/c9cp03650d.
36. Werle, C., et al., *Effect of Enhanced Electron Withdrawal on the Cohesion of Cr-Pd Hemichelates.* Eur. J. Inorg. Chem., 2019. **2019**(28): p. 3301-3308. 10.1002/ejic.201900450.
37. Kaya, Z., et al., *A Comparative Study of Confining Ligands Derived from Methylated Cyclodextrins in Gold-Catalyzed Cycloisomerization of 1,6-Enynes.* Eur. J. Org. Chem., 2019. **2019**(28): p. 4528-4537. 10.1002/ejoc.201900631.
38. Milovanovic, M.M., et al., *Investigation of interactions in Lewis pairs between phosphines and boranes by analyzing crystal structures from the Cambridge Structural Database.* Acta Crystallogr., Sect. B: Struct. Sci., Cryst. Eng. Mater., 2018. **74**(3): p. 255-263. 10.1107/s2052520618003736.
39. Kaya, Z., et al., *Benzimidazolium- and Benzimidazolilydene-Capped Cyclodextrins: New Perspectives in Anion Encapsulation and Gold-Catalyzed Cycloisomerization of 1,6-Enynes.* Chem. - Eur. J., 2018. **24**(68): p. 17921-17926. 10.1002/chem.201804710.
40. Binh, D.H., et al., *Entrapment of THF-Stabilized Iridacyclic Ir(III) Silylenes from Double H-Si Bond Activation and H_2 Elimination.* Chem. - Eur. J., 2018. **24**(66): p. 17577-17589. 10.1002/chem.201804048.
41. Dherbassy, Q., et al., *Two Stereoinduction Events in One C-H Activation Step: A Route towards Terphenyl Ligands with Two Atropisomeric Axes.* Angew. Chem., Int. Ed., 2018. **57**(17): p. 4668-4672. 10.1002/anie.201801130.
42. Hamdaoui, M., et al., *Iridacycles as Catalysts for the Autotandem Conversion of Nitriles into Amines by Hydrosilylation: Experimental Investigation and Scope.* Organometallics, 2017. **36**(24): p. 4864-4882. 10.1021/acs.organomet.7b00749.
43. Espinosa-Jalapa, N.A., et al., *Preparative resolution of stable enantio-enriched POCOP-based planar chiral pincer complexes.* J. Organomet. Chem., 2017. **845**: p. 125-134. 10.1016/j.jorganchem.2017.04.007.
44. Binh, D.H., et al., *Is the R_3Si Moiety in Metal-Silyl Complexes a Z ligand? An Answer from the Interaction Energy.* Chem. - Eur. J., 2017. **23**(67): p. 17058-17069. 10.1002/chem.201703373.
45. Jerhaoui, S., et al., *Stereoselective Sulfinyl Aniline-Promoted Pd-Catalyzed C-H Arylation and Acetoxylation of Aliphatic Amides.* Chem. - Eur. J., 2017. **23**(62): p. 15594-15600. 10.1002/chem.201703274.
46. Werle, C., et al., *Trans-cis C-Pd-C rearrangement in hemichelates.* Dalton Trans., 2017. **46**(25): p. 8125-8137. 10.1039/c7dt00872d.
47. Corre, Y., et al., *Efficient and Selective Hydrosilylation of Secondary and Tertiary Amides Catalyzed by an Iridium(III) Metallacycle: Development and Mechanistic Investigation.* ChemCatChem, 2017. **9**(11): p. 2009-2017. 10.1002/cctc.201700400.

48. Corre, Y., et al., *Regioselective hydrosilylation of terminal alkynes using pentamethylcyclopentadienyl iridium(III) metallacycle catalysts.* J. Mol. Catal. A: Chem., 2016. **423**: p. 256-263. 10.1016/j.molcata.2016.07.014.
49. Chetioui, S., et al., *Crystal structures of a copper(II) and the isotypic nickel(II) and palladium(II) complexes of the ligand (E)-1-[(2,4,6-tribromophenyl)diazenyl]naphthalen-2-ol.* Acta Crystallogr., Sect. E: Crystallogr. Commun., 2016. **72**(8): p. 1093-1098. 10.1107/s205698901601080x.
50. Hamdaoui, M., et al., *Evidence of a Donor-Acceptor (Ir-H)→SiR_3 Interaction in a Trapped Ir(III) Silane Catalytic Intermediate.* Organometallics, 2016. **35**(13): p. 2207-2223. 10.1021/acs.organomet.6b00248.
51. Schnee, G., et al., *Deprotonation of Al_2Me_6 by Sterically Bulky NHCs: Scope, Rationale through DFT Studies, and Application in the Methylenation of Carbonyl Substrates.* Organometallics, 2016. **35**(11): p. 1726-1734. 10.1021/acs.organomet.6b00159.
52. Mili, A., et al., *Chlorido{(E)-1-[(2-methoxyphenyl)diazenyl]naphthalen-2-olato}palladium(II).* IUCrData, 2016. **1**(4): p. x160691. 10.1107/s241431461600691x.
53. Petrovic, P., et al. *Non-covalent stabilization in transition metal coordination and organometallic complexes*. 2016. John Wiley & Sons, Inc.
54. Jerhaoui, S., et al., *Enantiopure Sulfinyl Aniline as a Removable and Recyclable Chiral Auxiliary for Asymmetric C(sp^3)-H Bond Activation.* Chem. - Eur. J., 2016. **22**(48): p. 17397-17406. 10.1002/chem.201603507.
55. Corre, Y., et al., *Selective hydrosilylation of esters to aldehydes catalyzed by iridium(III) metallacycles through trapping of transient silyl cations.* Chem. - Eur. J., 2016. **22**(39): p. 14036-14041. 10.1002/chem.201602867.
56. Anstine, D. and J.-P. Djukic. *Computational modeling and analysis of stable 14 electron hemichelated Pd-Cr complexes*. 2016. American Chemical Society.
57. Werle, C., et al., *New Pd(II) hemichelates devoid of incipient bridging CO···Pd interactions.* Dalton Trans., 2016. **45**(2): p. 607-617. 10.1039/c5dt03648h.
58. Chetioui, S., et al., *Crystal structure of bis{μ-1-[(E)-(3-methoxyphenyl)diazenyl]naphthalen-2-olato-κ3N2,O:O}bis({1-[(E)-(3-methoxyphenyl)diazenyl]naphthalen-2-olato-κ2N2,O}copper(II)).* Acta Crystallogr., Sect. E: Crystallogr. Commun., 2015. **71**(12): p. m211. 10.1107/s2056989015020824.
59. Werle, C., et al., *Stabilization of an Electron-Unsaturated Pd(I)-Pd(I) Unit by Double Hemichelation.* Organometallics, 2015. **34**(12): p. 3055-3064. 10.1021/acs.organomet.5b00349.