

List of publications – Dr. Christophe Werlé

2020

- Chatterjee, B., Chang, W.-C., **Werlé, C.** (2020). Molecularly Controlled Catalysis – Targeting Synergies Between Local and Non-local Environments *ChemCatChem* <https://doi.org/10.1002/cctc.202001431>
- Chatterjee, B., Chang, W.-C., Jena, S., **Werlé, C.** (2020). Implementation of Cooperative Designs in Polarized Transition Metal Systems—Significance for Bond Activation and Catalysis *ACS Catalysis* 10(23), 14024-14055. <https://doi.org/10.1021/acscatal.0c03794>
- Cramer, H.H., Chatterjee, B., Weyhermüller, T., **Werlé, C.**, Leitner, W. (2020). Controlling the Product Platform of Carbon Dioxide Reduction: Adaptive Catalytic Hydrosilylation of CO₂ Using a Molecular Cobalt(II) Triazine Complex *Angewandte Chemie International Edition* 59(36), 15674-15681. <https://doi.org/10.1002/anie.202004463>
- Erken, C., Hindemith, C., Weyhermüller, T., Hölscher, M., **Werlé, C.**, Leitner, W. (2020). Hydroamination of Aromatic Alkynes to Imines Catalyzed by Pd(II)–Anthraphos Complexes *ACS Omega* 5(15), 8912-8918. <https://doi.org/10.1021/acsomega.0c00562>

2019

- Martínez-Ferraté, O., Chatterjee, B., **Werlé, C.**, Leitner, W. (2019). Hydrosilylation of carbonyl and carboxyl groups catalysed by Mn(I) complexes bearing triazole ligands *Catalysis Science & Technology* 9(22), 6370-6379. <https://doi.org/10.1039/c9cy01738k>
- Chang, H.-C., Lin, Y.-H., **Werlé, C.**, Neese, F., Lee, W.-Z., Bill, E., Ye, S. (2019). Conversion of a Fleeting Open-Shell Iron-Nitride to an Iron-Nitrosyl *Angewandte Chemie International Edition* 58(49), 17589-17593. <https://doi.org/10.1002/anie.201908689>
- Rohner, S.S., Kinzel, N., **Werlé, C.**, Leitner, W. (2019). Systematic ligand variation to modulate the electrochemical properties of iron and manganese complexes *Dalton Transactions* 48(35), 13205-13211. <https://doi.org/10.1039/c9dt01343a>
- **Werlé, C.**, Karmazin, L., Bailly, C., Djukic, J.-P. (2019). Effect of Enhanced Electron Withdrawal on the Cohesion of Cr-Pd Hemichelates *European Journal of Inorganic Chemistry* 2019(28), 3301-3308. <https://doi.org/10.1002/ejic.201900450>
- **Werlé, C.**, Meyer, K. (2019). Organometallic Electrochemistry: Redox Catalysis Going the Smart Way *Organometallics* 38(6), 1181-1185. <https://doi.org/10.1021/acs.organomet.9b00111>
- **Werlé, C.**, Bailly, C., Karmazin, L., Djukic, J.-P. (2019). M-Carbonyl-bis(carbonyl{ η^5 -[tricarbonyl(η^6 -2-methylindenyl)chromium(0)]rhodium(III)}})(Rh-Rh) *IUCRData* 4, x190573. <https://doi.org/10.1107/S241431461900573X>

2018

- Erken, C., Kaithal, A., Sen, S., Weyhermüller, T., Hölscher, M., **Werlé, C.**, Leitner, W. (2018). Manganese-catalyzed hydroboration of carbon dioxide and other challenging carbonyl groups *Nature Communications* 9, 4521. <https://doi.org/10.1038/s41467-018-06831-9>
- Martínez-Ferraté, O., **Werlé, C.**, Franciò, G., Leitner, W. (2018). Aminotriazole Mn(I) Complexes as Effective Catalysts for Transfer Hydrogenation of Ketones *ChemCatChem* 23, 4514-4518. <https://doi.org/10.1002/cctc.201800953>

- Tindall, D.J., **Werlé, C.**, Goddard, R., Philipps, P., Farès, C., Fürstner, A. (2018). Structure and Reactivity of Half-Sandwich Rh(+3) and Ir(+3) Carbene Complexes. Catalytic Metathesis of Azobenzene Derivatives *Journal of the American Chemical Society* 140(5), 1884-1893. <https://doi.org/10.1021/jacs.7b12673>

2017

- **Werlé, C.**, Yin, C.-J.M., Heinemann, F.W., Hauser, C., Meyer, K. (2017). Synthesis and structural characterization of a highly substituted triazine ring comprising a sterically flexible methylene linker and coordinating substituents *Tetrahedron* 58(28), 2715-2719. <https://doi.org/10.1016/j.tetlet.2017.05.083>
- **Werlé, C.**, Dohm, S., Bailly, C., Karmazin, L., Ricard, L., Sieffert, N., Pfeffer, M., Hansen, A., Grimme, S., Djukic, J.-P. (2017). *trans-cis* C–Pd–C rearrangement in hemichelates *Dalton Transactions* 46(25), 8125-8137. <https://doi.org/10.1039/c7dt00872d>

2016

- Corre, Y., **Werlé, C.**, Brelot-Karmazin, L., Djukic, J.-P., Agbossou-Niedercorn, F., Michon, C. (2016). Regioselective hydrosilylation of terminal alkynes using pentamethylcyclopentadienyl iridium(III) metallocycle catalysts *Journal of Molecular Catalysis A: Chemical* 423, 256-263. <https://doi.org/10.1016/j.molcata.2016.07.014>
- **Werlé, C.**, Goddard, R., Philipps, P., Farès, C., Fürstner, A. (2016). Stabilization of a Chiral Dirhodium Carbene by Encapsulation and a Discussion of the Stereochemical Implications *Angewandte Chemie International Edition* 128(36), 10918-10923. <https://doi.org/10.1002/ange.201605502>
- **Werlé, C.**, Goddard, R., Philipps, P., Farès, C., Fürstner, A. (2016). Structures of Reactive Donor/Acceptor and Donor/Donor Rhodium Carbenes in the Solid State and Their Implications for Catalysis *Journal of the American Chemical Society* 138(11), 3797-3805. <https://doi.org/10.1021/jacs.5b13321>
- **Werlé, C.**, Anstine, D.M., Karmazin, L., Bailly, C., Ricard, L., Djukic, J.-P. (2016). New Pd(II) hemichelates devoid of incipient bridging CO...Pd interactions *Dalton Transactions* 45(2), 607-617. <https://doi.org/10.1039/c5dt03648h>

2015

- **Werlé, C.**, Goddard, R., Fürstner, A. (2015). The First Crystal Structure of a Reactive Dirhodium Carbene Complex and a Versatile Method for the Preparation of Gold Carbenes by Rhodium-to-Gold Transmetalation *Angewandte Chemie International Edition* 54(51), 15452-15456. <https://doi.org/10.1002/anie.201506902>
- Lima Barbosa, A.S., **Werlé, C.**, Colunga, C.O.O., Rodrigues, C.F., Toscano, R.A., Le Lagadec, R., Pfeffer, M. (2015). Further Insight into the Lability of MeCN Ligands of Cytotoxic Cycloruthenated Compounds: Evidence for the Antisymbiotic Effect Trans to the Carbon Atom at the Ru Center *Inorganic Chemistry* 54(15), 7617-7626. <https://doi.org/10.1021/acs.inorgchem.5b01236>

- **Werlé, C.**, Karmazin, L., Bailly, C., Ricard, L., Djukic, J.-P. (2015). Stabilization of an Electron-Unsaturated Pd(I)–Pd(I) Unit by Double Hemichelation *Organometallics* 34(12), 3055-3064. <https://doi.org/10.1021/acs.organomet.5b00349>

2014

- Hansen, A., Bannwarth, C., Grimme, S., Petrović, P., **Werlé, C.**, Djukic, J.-P. (2014). The Thermochemistry of London Dispersion-Driven Transition Metal Reactions: Getting the ‘Right Answer for the Right Reason’ *ChemistryOPEN* 3(5), 177-189. <https://doi.org/10.1002/open.201402017>
- **Werlé, C.**, Bailly, C., Karmazin-Brelot, L., Le Goff, X.-F., Pfeffer, M., Djukic, J.-P. (2014). First Stabilization of 14-Electron Rhodium(I) Complexes by Hemichelation *Angewandte Chemie International Edition* 53(37), 9827-9831. <https://doi.org/10.1002/anie.201405240>
- **Werlé, C.**, Le Goff, X.-F., Djukic, J.-P. (2014). Unusual outcome of the thermolytic condensation of diazoarylmethanes with a [tricarbonyl(η^6 -2-*p*-tolyl)chromium] 2-oxazolyl chelate of tetra carbonylrhenium *Journal of Organometallic Chemistry* 751, 754-759. <https://doi.org/10.1016/j.jorganchem.2013.07.070>

2013

- **Werlé, C.**, Bailly, C., Karmazin-Brelot, L., Le Goff, X.-F., Ricard, L., Djukic, J.-P. (2013). Hemichelation, a Way To Stabilize Electron-Unsaturated Complexes: The Case of T-Shaped Pd and Pt Metallacycles *Journal of the American Chemical Society* 135(47), 17839-17852. <https://doi.org/10.1021/ja4076327>
- **Werlé, C.**, Hamdaoui, M., Bailly, C., Le Goff, X.-F., Brelot, L., Djukic, J.-P. (2013). Electron-Deficient η^1 -Indenyl, η^3 -allylpalladium(II) Complexes Stabilized by Fluxional Non-covalent Interactions *Journal of the American Chemical Society* 135(5), 1715-1718. <https://doi.org/10.1021/ja312003q>