

- TC198** Reaction of Spiro[2.4]hepta-4,6-diene with Molybdenum(II) Indenyl Compounds: Effects of Substitution in the Indenyl Ligand  
J. Honzicek, C. C. Romão, M. J. Calhorda, A. Mukhopadhyay, J. Vinklerek, Z. Padelkova  
*Organometallics* **30**, 717-725 (2011) DOI: 10.1021/om100840r
- TC199** Chemoselective sulfide and sulfoxide oxidations by CpMo(CO)<sub>3</sub>Cl/HOOR: a DFT mechanistic study  
L. F. Veiros, C. A. Gamelas, M. J. Calhorda, C. C. Romão  
*Organometallics* **30**, 1454–1465 (2011)
- TC200** Synthesis and properties of Mo(II) complexes with *N*-heterocyclic ligands  
S. Quintal, S. Fedi, J. Barbetti, P. Pinto, V. Félix, M. G. B. Drew, P. Zanello, M. J. Calhorda  
*J. Organomet. Chem.* **696**, 2142-2152 (2011) doi:10.1016/j.jorganchem.2010.11.024
- TC201** Synthesis of Tetrahydronaphthalene Lignan Esters by Intramolecular Cyclization of Ethyl *p*-Azidophenyl-2-phenylalkanoates and Evaluation of the Growth Inhibition of Human Tumor Cell Lines  
O. Pinto, J. Sardinha, P. Vaz, F. Piedade, M. J. Calhorda, R. Abramovitch, N. Nazareth, M. S. J. Nascimento, M. Pinto, A. P. Rauter  
*J. Med. Chem.* **54**, 3175-3187 (2011) DOI: 10.1021/jm101182s
- TC202** A novel application of mesoporous silica material for extraction of pesticides  
A. S. Barreto, A. Aquino, S.C.S. Silva, M. E. Mesquita, M. J. Calhorda, M.S. Saraiva, S. Navickiene  
*Mat. Letters*, **65**, 1357-1359 (2011)
- TC203** Benzene and Heterocyclic Rings Formation in Cycloaddition Reactions Catalyzed by RuCp Derivatives: DFT Studies  
M. J. Calhorda, P. J. Costa, K. Kirchner  
*Inorg.Chim. Acta* **374**, 24-35 (2011)
- TC204** Indenyl effect in dissociative reactions. Nucleophilic substitution in iron carbonyl complexes: a case study.  
M. J. Calhorda, L. F. Veiros  
*Dalton Trans.* **40**, 11138 – 11146 (2011) DOI: 10.1039/C1DT00010A
- TC205** Coordination-driven self-assembly of thiocyanate complexes of Co(II), Ni(II) and Cu(II) with picolinamide: a structural and DFT study  
M. Đaković, D. Vila-Viçosa, M. J. Calhorda, Z. Popović  
*Cryst. Eng. Comm.* **13** (2011) 5863 – 5871 DOI: 10.1039/C1CE05332A
- TC206** Indenyl ring slippage in crown thioether complexes [IndMo(CO)<sub>2</sub>L]<sup>+</sup> and C-S Activation of Trithiacyclononane: Experimental and Theoretical Studies  
C. A. Gamelas, N. A. G. Bandeira, C. C. L. Pereira, M. J. Calhorda, E. Herdtweck, M. Machuqueiro, C. C. Romão, L. F. Veiros  
*Dalton Trans.* **40** (2011) 10513-10525 DOI: 10.1039/C1DT10607D
- TC207** Pyridine carboxylate complexes of Mo(II) as active catalysts in homogeneous and heterogeneous olefin epoxidation  
M. Vasconcellos-Dias, S. R. M. M. de Aguiar, C. D. Nunes, P. D. Vaz, T. G. Nunes, M. J. Calhorda  
*Curr. Inorg. Chem.* **1** (2011) 146-155
- TC208** Reversible Addition of CO to Coordinatively Unsaturated High-Spin Iron(II) Complexes  
C. Holzhaecker, C. M. Standfest-Hauser, M. Puchberger, K. Mereiter, L. F. Veiros, M. J. Calhorda, M. D. Carvalho, L. P. Ferreira, M. Godinho, F. Hartl, and K. Kirchner  
*Organometallics* **30** (2011) 6587 – 6601 DOI: 10.1021/om200711q

- TC209** Unveiling the Mechanisms of Catalytic Oxidation Reactions Mediated by Oxo-Molybdenum Complexes: A Computational Overview  
M. J. Calhorda, P. J. Costa  
*Curr. Org. Chem.* 16 (2012) 65-72.
- TC210** Electronic structure and properties of camphorimine Cu(I) coordination polymers  
M. F. N. N. Carvalho, T. A. Fernandes, A. M. Galvão, N. A. G. Bandeira, M. J. Calhorda, A. M. Botelho do Rego  
*J. Pol. Sci. Part A: Pol. Chem.* 50 (2012) 1102-1110 DOI: 10.1002/pola.25866
- TC211** The influence of crystal packing on *cis-trans* isomerism in nickel(II) complexes with 3-hydroxypicolinic acid and on type of coordination polyhedron in copper(II) complexes  
B.-M. Kukovec, P. D. Vaz, M. J. Calhorda, Z. Popović  
*Polyhedron* 39 (2012) 66-75.
- TC212** Syntheses and photophysical properties of new iminopyrrolyl boron complexes and their application in efficient single-layer non-doped OLEDs prepared by spin coating  
D. Suresh, C. S. B. Gomes, P. T. Gomes, R. E. Di Paolo, A. L. Maçanita, M. J. Calhorda, A. Charas, J. Morgado and M. T. Duarte  
*Dalton Trans.* 41 (2012) 8502–8505 DOI: 10.1039/C2DT30487B
- TC213** 1,1'-Bis(diphenylphosphino)ferrocene bridging two mono(cyclopentadienyl) cobalt moieties: synthesis, structure, electrochemistry and DFT studies  
V. Rosa, S. Realista, A. Mourato, L. M. Abrantes, J. Henriques, M. J. Calhorda, T. Avilés, M. G. B. Drew, V. Félix  
*J. Organomet. Chem.* 712 (2012) 52-56 DOI: 10.1016/j.jorganchem.2012.04.012
- TC214** An Oligosilsesquioxane Cage Functionalized with Molybdenum(II) Organometallic Fragments  
N. L. Dias Filho, F. C. M. Portugal, J. M. F. Nogueira, P. Brandão, V. Félix, P. D. Vaz, Carla D. Nunes, L. F. Veiros, M. J. Villa de Brito, and M. J. Calhorda  
*Organometallics* 31 (2012) 4495–4503 <http://dx.doi.org/10.1021/om3003043>.
- TC215** Electronic structure of ytterbium bis -indenyl and -cyclopentadienyl  $\alpha$ -diimines complexes: a DFT and MS-CASPT2 investigation  
N. A. G. Bandeira, C. Daniel, A. Trifonov, M. J. Calhorda  
*Organometallics* 31 (2012) 4693–4700 DOI: 10.1021/om300081j
- TC216** Photophysical properties of iminopyrrolyl boron complexes: a DFT interpretation  
M. J. Calhorda, D. Suresh, P. T. Gomes, R. E. Di Paolo, A. L. Maçanita  
*Dalton Trans.* 41 (2012) 13210 – 13217 DOI:10.1039/C2DT31104F.
- TC217** Charge parametrization of the DvH-c3 heme group: validation using constant-(pH,E) molecular dynamics simulations.  
J. Henriques, P. Costa, M. J. Calhorda, M. Machuqueiro  
*J. Phys. Chem.* 116 (2012) 8812 – 8821
- TC218** Tris(organotin)tungstogermanate, a Sandwich Organometallic Derivative of a Keggin type polyoxometalate: Synthesis and DFT study  
H. Liu, N. A. G. Bandeira, V. Félix, M. J. Calhorda  
*Eur. J. Inorg. Chem.* (2013) 1713 – 1719.
- TC219** Mo(II) complexes of 8-aminoquinoline and their immobilization in MCM-41  
M. S. Saraiva, C.D. Nunes, T. G. Nunes, M. J. Calhorda  
*J. Appl. Cat. A* 455 (2013) 172 – 182.

- TC220** Cytotoxicities of Polysubstituted Chlorodicarbonyl(cyclopentadienyl) and (Indenyl)ruthenium Complexes  
D. Mavrynsky, J. Rahkila, D. Bandarra, S. Martins, M. Meireles, M.J. Calhorda, I. J. Kovács, I. Zupkó, M. M. Hänninen and R. Leino  
*Organometallics* **32** (2013) 3012-3017.
- TC221** Towards the understanding of radical reactions: experimental and computational studies of titanium(III) diamine bis(phenolate) complexes  
S. Barroso, F. Madeira, M. J. Calhorda, M. J. Ferreira, M. T. Duarte and A. M. Martins  
*Inorg. Chem.* **52** (2013) 9427–9439 DOI: 10.1021/ic401008y
- TC222** Self-assembly of copper(II) picolinamide building blocks: synthesis and mechanism  
M. Đaković, D. Vila-Viçosa, M. J. Calhorda, N. A. G. Bandeira, B. Kozlevčar, Z. Jagličić, Z. Popović  
*Cryst. Eng. Comm.* **15**, 2013, 8074-8087 DOI: 10.1039/C3CE41011K
- TC223** New Mo(II) complexes in MCM-41 and silica: Synthesis and catalysis  
M. S. Saraiva, C. I. Fernandes, T. G. Nunes, C. D. Nunes, M. J. Calhorda  
*J. Organomet. Chem.* **751**, 2014, 443-452. <http://dx.doi.org/10.1016/j.jorganchem.2013.07.081>
- TC224** Unveiling the dual role of the cholinium hexanoate ionic liquid as solvent and catalyst in suberin depolymerisation  
R. Ferreira, H. Garcia, A. F. Sousa, M. Guerreiro, F. J. S. Duarte, C. S. R. Freire, M. J. Calhorda, A. J. D. Silvestre, W. Kunz, L. P. N. Rebelo, C. da Silva Pereira  
*RSC Adv.* **3**, 2014, 2993-3002. DOI: 10.1039/C3RA45910A, Paper
- TC225** Solvent-Dependent Formation of Os(0) Complexes by Electrochemical Reduction of [Os(CO)(bpy)(L)Cl<sub>2</sub>] (bpy = 2,2'-bipyridine; L = Cl<sup>-</sup>, PrCN)  
J. Tory, L. King, A. Maroulis, M. Haukka, M. J. Calhorda and F. Hartl  
*Inorg. Chem.* **53**, 2014, 1382-1396. DOI: 10.1021/ic402146t
- TC226** Tunable Fluorophores based on 2-(*N*-Arylimino)pyrrolyl Chelates of Diphenylboron: Synthesis, Structure, Photophysical Characterization and Application in OLEDs  
D. Suresh, P. S. Lopes, B. Ferreira, C. A. Figueira, C. S. B. Gomes, P. T. Gomes, R. E. Di Paolo, A. L. Maçanita, M. T. Duarte, A. Charas, J. Morgado, M. J. Calhorda  
*Chem. Eur. J.* **20**, 2014, 4126-4140. DOI: 10.1002/chem.201303607
- TC227** Dinuclear Zinc *N*-heterocyclic Carbene Complexes for either the Controlled ROP of lactide or the Controlled Degradation of Polylactide Under Mild Conditions  
C. Fliedel, D. Vila-Viçosa, M. J. Calhorda, S.I Dagorne, T. Avilés  
*ChemCatChem* **6**, 2014, 1357-1367. DOI: 10.1002/cctc.201301015
- TC228** One-Electron Oxidation of ReCp(CO)<sub>2</sub>L (L = PPh<sub>3</sub>, η<sup>2</sup>-2-butene, η-diphenylacetylene): Electrochemical, Spectroscopic and Computational Studies of the Electronic Properties and Dimerization Tendencies of 17-Electron Rhenium Complexes  
D. Chong, V. H. Teixeira, M. J. Calhorda, W. E. Geiger  
*Organometallics* **33**, 2014, 4706–4715. DOI: 10.1021/om401198j
- TC229** Six-Coordinate High-Spin Iron(II) Complexes with Bidentate PN Ligands based on 2-Aminopyridine – New Fe(II) Spin Crossover Systems<sup>†</sup>  
C. Holzhaecker, M. J. Calhorda, A. Gil, M. D. Carvalho, L. P. Ferreira, B. Stöger, K. Mereiter, M. Weil, D. Müller, P. Weinberger, E. Pittenauer, G. Allmaier, K. Kirchner  
*Dalton Trans.* **43**, 2014, 11152-11164. DOI: 10.1039/c4dt00186a

- TC230** Successful oxidation of  $\text{Ph}_2\text{P}(\text{CH}_2)_n\text{PPh}_2$  ( $n = 2, 4, 6$ ) by tellurium leading to  $\text{Ph}_2\text{P}(\text{Te})(\text{CH}_2)_n\text{P}(\text{Te})\text{Ph}_2$   
L. Jeremias, M. Babiak, V. Kubát, M.J. Calhorda, Z. Trávníček, J. Novosad  
*RSC Adv.* **4**, 2014, 15428-15430. DOI: 10.1039/C4RA00157E, Communication
- TC231** CNN Pincer Ruthenium Catalysts for Transfer and  $\text{H}_2$  Hydrogenation of Ketones: Experimental and Computational Studies  
W. Baratta, M. J. Calhorda, P. J. Costa, G. Esposito, E. Herdtweck, S. Magnolia, C. Mealli, A. Messaoudi, S. A. Mason, L. F. Veiros  
*Chem. Eur. J.* **20**, 2014, 13603-13617 DOI: 10.1002/chem.201402229
- TC232** Four- and five-coordinate high-spin iron(II) complexes bearing bidentate soft/hard SN ligands based on 2-aminopyridine  
C. Holzhaecker, M. J. Calhorda, A. Gil, M. D. Carvalho, L. P. Ferreira, K. Mereiter, B. Stöger, E. Pittenauer, G. Allmaier, K. Kirchner  
*Polyhedron* **81**, 2014, 45–55. <http://dx.doi.org/10.1016/j.poly.2014.05.052>
- TC233** Cationic Half-Sandwich Iron(II) and Iron(III) Complexes with N-Heterocyclic Carbene Ligands  
J.M.S. Cardoso, A. Fernandes, B.P. Cardoso, M.D. Carvalho, L.P. Ferreira, M.J. Calhorda, B. Royo  
*Organometallics* **33**, 2014, 5670–5677. DOI: 10.1021/om500528p
- TC234** Influence of activated carbons porous structure on iopamidol adsorption  
A. S. Mestre, M. Machuqueiro, M. Silva, R. Freire, I. M. Fonseca, M. S. C. S. Santos, M. J. Calhorda, A. P. Carvalho  
*Carbon* **81**, 2014, 607-615. [doi.org/10.1016/j.carbon.2014.05.065](http://doi.org/10.1016/j.carbon.2014.05.065)
- TC235** Synthesis, Cytotoxic and Hydrolytic Studies of Titanium Complexes Anchored by a Tripodal Diamine Bis(phenolate) Ligand  
S. Barroso, A.M. Coelho, S. Gómez-Ruiz, M.J. Calhorda, Ž. Žižak, G. N. Kaluđerović, A.M. Martins  
*Dalton Trans.* **43**, 2014, 17422–17433. DOI: 10.1039/C4DT00975D
- TC236** Vanadyl cationic complexes as catalysts in olefin oxidation  
C. D. Nunes, P.D. Vaz, V. Félix, L. F. Veiros, T. Moniz, M. Rangel, S. Realista, A. C. Mourato, M. J. Calhorda  
*Dalton Trans.* **44**, 2015, 5125–5138. DOI: 10.1039/C4DT03174A
- TC237** Pore size matters! Helical heterogeneous catalysts in olefin oxidation  
M.S. Saraiva, C.I. Fernandes, T.G. Nunes, M.J. Calhorda, C.D. Nunes  
*Appl. Catal. A* **180**, 2015, 130–140 [dx.doi.org/10.1016/j.apcata.2015.01.040](http://dx.doi.org/10.1016/j.apcata.2015.01.040)
- TC238** Molybdenum(II) catalyst precursors in olefin oxidation reactions  
C.D. Nunes, M. J. Calhorda  
*Inorg. Chim. Acta* **431**, 2015, 122–131.  
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- TC239** Fe(III) SalEen derived Schiff base complexes as potential contrast agents  
B. P. Cardoso, A. I. Vicente, J. B. J Ward, P. J. Sebastião, F. V. Chávez, S. Barroso, A. Carvalho, S. J. Keely, P. N. Martinho, Maria José Calhorda  
*Inorg. Chim. Acta* **432**, 2015, 258-266.  
<http://dx.doi.org/10.1016/j.ica.2015.04.026>
- TC240** Asymmetric Binuclear Ni(II) And Cu(II) Schiff Base Metallopolymers  
S. Realista, A. S. Viana, B. P. Cardoso, A. M. Botelho do Rego, P. D. Vaz, A. I. Melato, P. N. Martinho, M. J. Calhorda  
*RSC Adv.* **5**, 2015, 39495-39504.

**TC241** Comparing spectroscopic and electrochemical properties of complexes of type  $[\text{Cp}'\text{M}(\eta^3\text{-C}_3\text{H}_5)(\text{CO})_2]$  ( $\text{Cp}' = \text{Cp, Ind, Flu}$ ;  $\text{M} = \text{Mo, W}$ ): a complementary experimental and DFT study  
I. S. Gonçalves, L. F. Veiros, C. A. Gamelas, C. Cabrita, M. J. Calhorda, C. F. G. C. Geraldes, J. Green, E. Packham, M. G. B. Drew, V. Félix, A. G. Santos, C. C. Romão  
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**TC242** Preference for sulfoxide S- or O-bonding to 3d transition metals – DFT insights  
B.P. Cardoso, B. Royo, M. J. Calhorda  
*J. Organomet. Chem.* **792**, 2015, 167-176.  
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**TC243** Catalytic activity of Mo(II) complexes in homogeneous and heterogeneous conditions  
Maria Vasconcellos Dias, Marta S. Saraiva, Paula Ferreira, and Maria José Calhorda  
*Organometallics* **34**, 2015, 1465-1478 doi: 10.1021/om501068q

**TC244** Luminescent Di- and Trinuclear Boron Complexes Based on Aromatic Iminopyrrolyl Spacer Ligands: Synthesis, Characterization and Application in OLEDs  
D. Suresh, C. S. B. Gomes, P. S. Lopes, C. A. Figueira, B. Ferreira, P. T. Gomes, R. E. Di Paolo, A. L. Maçanita, M. T. Duarte, A. Charas, J. Morgado, D. Vila-Viçosa, M. J. Calhorda  
*Chem. Eur. J.* **21**, 2015, 9133-9149 DOI: 10.1002/chem.201500109

**TC245** How the Intercalation of Phenanthroline Affects the Structure, Energetics and Bond Properties of DNA Base Pairs. Theoretical Study Applied to Adenine-Thymine and Guanine-Cytosine Tetramers  
A. Gil, V. Branchadell, M.J. Calhorda  
*J. Chem. Theory Comput.* **11**, 2015, 2714–2728 DOI: 10.1021/ct5006104

**TC246** Synthesis and Reactivity of Taddol-Based Chiral Fe(II) PNP Pincer Complexes -Solution Equilibria between  $\kappa^2\text{P,N-}$  and  $\kappa^3\text{P,N,P-}$  Bound PNP Pincer Ligands  
C. Holzhaecker, B. Stöger, M. D. Carvalho, L. P. Ferreira, E. Pittenauer, G. Allmaier, L. F. Veiros, S. Realista, A. Gil, M. J. Calhorda, D. Müller, K. Kirchner  
*Dalton Trans.* **44**, 2015, 13071–13086

**TC247** Wittig Reaction: Domino Olefination and Stereoselectivity DFT Study. Synthesis of the Miharamycins' Bicyclic Sugar Moiety  
V. Cachatra, A. Almeida, J. Sardinha, S. D. Lucas, A. Gomes, P. D. Vaz, M. H. Florêncio, R. Nunes, D. Vila-Viçosa, M. J. Calhorda, A. P. Rauter  
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