

- TC143** Synthesis, Structural Characterization and Theoretical Studies of Gold(I) and Gold(I)-Gold(III) Thiolate Complexes: Quenching of Gold(I) Thiolate Luminescence  
M. Bardají, M. J. Calhorda, P. J. Costa, P. G. Jones, A. Laguna, M. Reyes Pérez, M. D. Villacampa  
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- TC144** Olefin epoxidation with *tert*-Butyl Hydroperoxide catalyzed by MoO<sub>2</sub>X<sub>2</sub>L complexes - A DFT mechanistic study  
L. F. Veiros, Â. Prazeres, P. J. Costa, C. C. Romão, F. E. Kühn, M. J. Calhorda  
*Dalton Transactions* 1383-1389 (2006).
- TC145** A DFT and MP2 study of luminescence of gold(I) complexes  
P. J. Costa and M. J. Calhorda  
*Inorg. Chim. Acta* **359**, 3617-3624 (2006).
- TC146** Structural preferences of cyclopentadienyl and indenyl rings in iridium(I) carbene complexes  
M. Prinz, L. F. Veiros, M. J. Calhorda, C. C. Romão, E. Herdtweck, F. Kühn, W. H. Herrmann  
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- TC147** Formation of Pyridine from Acetylenes and Nitriles Catalyzed by RuCpCl, CoCp, and RhCp derivatives - A Computational Mechanistic Study  
G. Dazinger, M. Torres-Rodriguez, K. Kirchner, M. J. Calhorda  
*J. Organomet. Chem.* **691**, 4434-4445 (2006).
- TC148** Heptacoordinate Halocarbonyl Molybdenum(II) and Tungsten(II) Complexes as Heterogeneous Polymerization Catalysts  
J. Gimenez, C. D. Nunes, P. D. Vaz, A. A. Valente, P. Ferreira and M. J. Calhorda  
*J. Mol. Cat. A Chemical* **256**, 90-98 (2006).
- TC149** Synthesis and Characterisation of hybrid mesoporous materials with the 1,4-diazobutadiene ligand  
C. D. Nunes, P. D. Vaz, P. Brandão, J. Rocha, P. Ferreira, N. Bion, M. J. Calhorda  
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- TC150** Group 11 Complexes with the bis(3,5-dimethylpyrazol-1-yl)methane ligand. How secondary bonds can influence the coordination environment of Ag(I): the role of coordinated water in [Ag<sub>2</sub>(μ-L<sub>2</sub>)(OH<sub>2</sub>)<sub>2</sub>](OTf)<sub>2</sub>.  
M. J. Calhorda, P. J. Costa, O. Crespo, M. C. Gimeno, P. G. Jones, A. Laguna, M. Naranjo, S. Quintal, Y.-J. Shi, M. D. Villacampa  
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- TC151** New polynuclear Mo-Fe complexes with Ferrocenylamidobenzimidazole ligands  
P. N. Martinho, S. Quintal, P. Costa, S. Losi, V. Félix, M. C. Gimeno, A. Laguna, M. G. B. Drew, P. Zanello, M. J. Calhorda  
*European Journal of Inorganic Chemistry* 4096-4103 (2006)
- TC152** Synthesis and Ligand Properties towards Gold and Silver of the Ferrocenylamidobenzimidazole Ligand  
M. J. Calhorda, P. J. Costa, P. N. Martinho, M. C. Gimeno, A. Laguna, S. Quintal, M. D. Villacampa  
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- TC153** High Yield Ruthenium Catalysed Friedel-Crafts Type Allylation Reactions Using Ru(IV) Dicationic Catalysts  
I. Fernández, R. Hermatschweiler, F. Breher, P. S. Pregosin, L. F. Veiros, M. J. Calhorda  
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- TC154** Diffusion and Overhauser NMR studies on dicationic palladium complexes of BINAP  
D. Nama, D. Schott, P. S. Pregosin, L. F. Veiros, M. J. Calhorda  
*Organometallics* **25**, 4596-4604 (2006).
- TC155** Ring slippage vs. charge transfer in the reductive chemistry of [IndMo(CO)<sub>2</sub>( $\alpha$ -diimine)]<sup>+</sup> cations  
C. C. L. Pereira, P. J. Costa, M. J. Calhorda, A. C. Freire, S. S. Rodrigues, E. Herdtweck, C. C. Romão  
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- TC156** The photochemistry of methyltrioxorhenium revisited: a DFT/TD-DFT and CASSCF/MS-CASPT2 theoretical study  
P. J. Costa, M. J. Calhorda, J. Bossert, C. Daniel, C. C. Romão  
*Organometallics* **25**, 5235-5241 (2006).
- TC157** Electrochemical Oxidation of [CoCpCo(CO)<sub>2</sub>]: Reaction of a 17 e<sup>-</sup>/ 18 e<sup>-</sup> Pair and Production of a Unique Dimer Radical  
A. Nafady, P. J. Costa, M. J. Calhorda, W. E. Geiger  
*J. Am. Chem. Soc.* **128**, 16587-16599 (2006)
- TC158** Immobilization and Delivery of Sertraline using Inorganic Micro and Mesoporous Materials  
C. D. Nunes, P. D. Vaz, A. C. Fernandes, P. Ferreira, C. C. Romão, M. J. Calhorda  
*Eur. J. Pharm. Biopharm.* **66**, 357-365 (2007)
- TC159** Catalyzing aldehyde hydrosilylation with a Mo(VI) complex: a DFT study  
P. J. Costa, C. C. Romão, A. C. Fernandes, B. Royo, P. M. Reis, M. J. Calhorda  
*Chemistry Eur. Journal* **13**, 3934 -3941 (2007)
- TC160** Geometry optimisation of a Ru(IV) allyl dicationic complex: a DFT failure?  
M. J. Calhorda, P. S. Pregosin, L. F. Veiros  
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- TC161** A New Look at the Ylidic Bond in Phosphorous Ylides and Related Compounds: An Energy Decomposition Analysis Combined with a Domain-Averaged Fermi Hole Analysis  
M. J. Calhorda, A. Krapp, G. Frenking  
*J. Phys. Chem. A* **111**, 2859 - 2869 (2007)
- TC162** Pyridine carboxylate complexes of Mo(II) as active catalysts in homogeneous and heterogeneous polymerization  
M. Vasconcellos-Dias, C. D. Nunes, P. D. Vaz, P. Ferreira, M. J. Calhorda  
*Eur. J. Inorg Chem.* 2917-2925 (2007)
- TC163** Vibrational study on the local structure of post-synthetic and hybrid mesoporous materials – are there fundamental distinctions?  
P. D. Vaz, C. D. Nunes, M. Vasconcellos-Dias, M. M. Nolasco, P. J. A. Ribeiro-Claro, M. J. Calhorda  
*Chemistry Eur. J.* **13**, 7874 - 7882 (2007)
- TC164** Remote metal-arene  $\pi$  bonding in organometallic complexes: a DFT study  
P. J. Costa, M. José Calhorda, P. S. Pregosin  
*Coll. Czech. Chem. Comm.* **72**, 703-704 (2007)
- TC165** Can five-membered Te<sub>2</sub>N<sub>2</sub>S cycles be considered aromatic?  
N. A. G. Bandeira, C. Corminboeuf, M. J. Calhorda  
*Struct.Chem.* **18**, 841 - 847 (2007)

- TC166** Hyper-electronic Metal-Carborane Analogues of Cymantrene Anions: Electronic and Structural Non-Innocence of the Tricarbadeboranyl Ligand  
A. Nafady, R. Butterick III, M. J. Calhorda, P. J. Carroll, D. Chong, W. E. Geiger, L. G. Sneddon  
*Organometallics* **26**, 4471 - 4482 (2007)
- TC167** Molybdenum  $\eta^3$ -allyldicarbonyl complexes as a new class of precursors for highly reactive epoxidation catalysts with *tert*-butyl hydroperoxide  
J. C. Alonso, P. Neves, M. J. Pires da Silva, S. Quintal, P. D. Vaz, C. Silva, A. A. Valente, P. Ferreira, M. J. Calhorda, V. Félix, M. G. B. Drew  
*Organometallics* **26**, 5548 - 5556 (2007)
- TC168** Immobilisation of  $\eta^3$ -allyldicarbonyl complexes of Mo(II) with bidentate nitrogen ligands into aluminium pillared clays  
J. C. Alonso, P. Neves, C. Silva, A. A. Valente, P. Brandão, S. Quintal, M. J. Brito, P. Pinto, V. Félix, M. G. B. Drew, J. Pires, A. P. Carvalho, M. J. Calhorda, P. Ferreira  
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- TC169** Synthesis and properties of new trinuclear Mo(II) complexes containing imidazole and benzimidazole ferrocene units  
S. Quintal, J. Matos, I. Fonseca, V. Félix, M. G. B. Drew, N. Trindade, M. Meireles, M. J. Calhorda  
*Inorg. Chim. Acta* **361**, 1584-1596 (2008)
- TC170** Synthesis and catalytic properties of manganese(II) and oxovanadium(IV) complexes anchored to mesoporous MCM-41  
T. A. Fernandes, C. D. Nunes, P. D. Vaz, M. J. Calhorda, P. Brandão, J. Rocha, I. S. Gonçalves, A. A. Valente, L. P. Ferreira, M. Godinho, P. Ferreira  
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- TC171** Synthesis and characterisation of organo-silica hydrophobic clay heterostructures for volatile organic compounds removal  
C. D. Nunes, J. Pires, A. P. Carvalho, M. J. Calhorda, P. Ferreira  
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- TC172** Mixed-Ligand Re Tricarbonyl Complexes Anchored on a ( $\kappa^2$ -H, S) Trihydro(mercaptoimidazolyl)borate: A Missing Binding Motif for Soft Scorpionates  
M. Videira, L. Maria, A. Paulo, I. C. Santos, I. Santos, P. D. Vaz, M. J. Calhorda  
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- TC173** The  $[\text{Re}(\square^5\text{-C}_5\text{H}_4\text{R})(\text{CO})_3]^+$  Family of 17-Electron Compounds: Monomer/Dimer Equilibria and Other Reactions  
D. Chong, D. R. Laws, A. Nafady, P. J. Costa, A. L. Rheingold, M. J. Calhorda, W. E. Geiger  
*J. Am. Chem. Soc.* **130**, 2692-2703 (2008). DOI: 10.1021/ja710513n
- TC174** Hydrogen activation by high-valent oxo-molybdenum(VI) and -rhenium(VII) and (V) compounds  
P. M. Reis, P. J. Costa, C. C. Romão, J. A. Fernandes, M. J. Calhorda, B. Royo  
*Dalton Trans.* 1727 - 1733 (2008)
- TC175** Heptacoordinate tricarbonyl Mo(II) complexes as highly selective oxidation homogeneous and heterogeneous catalysts  
M. Vasconcellos-Dias, C. D. Nunes, P. D. Vaz, P. Ferreira, P. Brandão, V. Félix, M. J. Calhorda  
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**TC176** Weak  $\eta^2$  olefin bonding in Pd and Pt allyl complexes containing chiral monodentate ligands with alpha-phenyl methyl amine side chains.

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**TC177** Photoinduced bond cleavage in  $\text{CH}_3\text{ReO}_3$ : excited states dynamics

P. J. Costa, M. J. Calhorda, S. Villaume, C. Daniel  
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**TC178** Pseudopolymorphism in nickel(II) complexes with 6-methylpicolinic acid. Synthesis, structural, spectroscopic, thermal and DFT study.

B.-M. Kukovec, Z. Popović, P. D. Vaz, M. J. Calhorda, K. Furić, G. Pavlović, M. R. Linarić  
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**TC179** Nitrogen donor ligands bearing N-H groups: effect on catalytic and cytotoxic activity of molybdenum  $\eta^3$ -allyldicarbonyl complexes

M. S. Saraiva, S. Quintal, F. C. M. Portugal, T. A. Lopes, V. Félix, J. M. F. Nogueira, M. Meireles, M. G. B. Drew, M. J. Calhorda  
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M. S. Saraiva, N. L. Dias Filho, C. D. Nunes, P. D. Vaz, T. G. Nunes, M. J. Calhorda  
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**TC181** Influence of the Ligand Donor Atoms on the *in vitro* Stability of Rhenium(I) and Technetium (I)-99m Complexes with Pyrazole-containing Chelators: Experimental and DFT Studies

C. Moura, C. Fernandes, L. Gano, A. Paulo, I. C. Santos, I. Santos, M. J. Calhorda  
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**TC182** Kinetic Studies on the Oxidation of  $\eta^5$ -Cyclopentadienyl Methyl Tricarbonyl Molybdenum(II) and the use of its Oxidation Products as Olefin Epoxidation Catalysts

A. Al-Ajlouni, D. Veljanovski, A. Capapé, J. Zhao, E. Herdtweck, M. J. Calhorda, F. E. Kühn  
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A. Nowak, M. J. Calhorda, P. J. Costa, S. Woodward  
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**TC184** Expanding the role of oxo-molybdenum(VI) catalysts: a DFT interpretation of X-H activation leading to reduction or oxidation

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**TC185** Soluble Redox-Active Polymetallic Chains  $[\{\text{Ru}^0(\text{CO})(\text{L})(\text{bpy})\}^m]_n$  (bpy = 2,2'-bipyridine, L = PrCN, Cl; m = 0, -1): Electrosynthesis and Characterization

F. Hartl, A. K. Renfrew, F. Lafolet, T. Mahabiersing, M. J. Calhorda, S. Chardon-Noblat, M. Haukka, A. Deronzier  
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**TC186**  $\text{MoO}_2\text{Cl}_2$  as a novel catalyst for C-P bond formation and for hydrophosphonylation of aldehydes

R. G. de Noronha, P. J. Costa, C. C. Romão, M. José Calhorda, A. C. Fernandes  
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- TC187** Synthesis, Structure and Photophysical Characterization of Blue-Green Luminescent Zinc Complexes Containing 2-Iminophenanthrolyl Ligands  
C. S. B. Gomes, P. T. Gomes, M. T. Duarte, R. E. Di Paolo, A. L. Maçanita, M. J. Calhorda  
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- TC188** Silver(I) and copper(I) complexes with ferrocenyl ligands bearing imidazole or pyridyl substituents  
S. Quintal, M. C. Gimeno, A. Laguna, M. J. Calhorda  
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- TC189** Striking Differences between the Solution and Solid-state Reactivity of Iron PNP Pincer Complexes with Carbon Monoxide  
D. Benito-Garagorri, L. G. Alves, M. Puchberger, K. Mereiter, L. F. Veiros, M. J. Calhorda, M. D. Carvalho, L. P. Ferreira, M. Godinho, K. Kirchner  
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- TC190** The role of Cp vs Ind in Mo(II) spirodiene complexes reactivity: a DFT mechanistic study  
L. F. Veiros, J. Honzík, C. C. Romão, M. J. Calhorda  
*Inorg. Chim. Acta* **363**, 555–561 (2010). doi:10.1016/j.ica.2009.03.029
- TC191** Olefin Epoxidation catalyzed by  $\eta^5$ -Cyclopentadienyl Molybdenum Compounds: a computational study  
P. J. Costa, M. J. Calhorda, F. E. Kühn  
*Organometallics* **29**, 303-311 (2010). DOI: 10.1021/om9002522
- TC192** The effect of immobilization on the catalytic activity of molybdenum  $\eta^3$ -allyldicarbonyl complexes with nitrogen donor ligands bearing N-H groups  
M. S. Saraiva, C. D. Nunes, T. G. Nunes, M. J. Calhorda  
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- TC193** Chemoselectivity as a Delineator of Cuprate Structure in Catalytic 1,4-Addition of Diorganozincs to Michael Acceptors  
M. Welker, S. Woodward, L. F. Veiros, M. J. Calhorda  
*Chem. Eur. J.* **16**, 5620-5629 (2010)
- TC194** Disappearing and concomitant polymorphism of nickel(II) complexes with 6-hydroxypicolinic acid. Structural and DFT studies  
B.-M. Kukovec, P. D. Vaz, M. J. Calhorda, Z. Popović  
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- TC195** Heteropolynuclear Gold Complexes with Metallophilic Interactions. Modulation of the Luminescent Properties  
M. J. Calhorda, C. Ceamanos, O. Crespo, M. C. Gimeno, A. Laguna, C. Larráz, P. D. Vaz, M. D. Villacampa  
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- TC196** Mo(II) complexes: a new family of cytotoxic agents?  
D. Bandarra, M. Lopes, T. Lopes, J. Almeida, M. S. Saraiva, M. Vasconcellos-Dias, C. D. Nunes, V. Félix, P. Brandão, M. Meireles, and M. J. Calhorda  
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- TC197** Highly Efficient Reduction of Sulfoxides with the System Borane/Oxo-rhenium Complexes  
A. C. Fernandes, J. A. Fernandes, C. C. Romão, L. F. Veiros, M. J. Calhorda  
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