

Publications list – Dr. Ragnar Björnsson – 2019-04

2019

- Barclay, M.; Björnsson, R.; Cipriani, M.; Terfort, A.; Fairbrother, H.; Ingólfsson, O. (2019) The role of the dihedral angle and excited cation states in ionization and dissociation of mono-halogenated biphenyls; a combined experimental and theoretical coupled cluster study. *Phys. Chem. Chem. Phys.*, *21*, 4556-4567.
- Thorhallsson, A. Th.; Björnsson, R. (2019), Computational mechanistic study of [MoFe₃S₄] cubanes for catalytic reduction of nitrogenase substrates. *Inorg. Chem.* *58*, 1886-1894.
- Sterling, C. M.; Björnsson, R. (2019) A Multi-Step Explicit Solvation Protocol for Calculation of Redox Potentials. *J. Chem. Theory Comput.*, *15*, 52-67.

2018

- Benediktsson, B.; Thorhallsson, A. T.; Björnsson, R., (2018) QM/MM calculations reveal a bridging hydroxo group in a vanadium nitrogenase crystal structure. *Chem. Comm.*, *54*, 7310-7313.
- P, R. K. T.; Weirich, P.; Hrachowina, L.; Hanefeld, M.; Björnsson, R.; Hrodmarsson, H. R.; Barth, S.; Fairbrother, D. H.; Huth, M.; Ingólfsson, O. *Beilstein* (2018) Electron interactions with the heteronuclear carbonyl precursor H₂FeRu₃(CO)₁₃ and comparison with HFeCo₃(CO)₁₂: from fundamental gas phase and surface science studies to focused electron beam induced deposition. *J. Nanotechnol.*, *9*, 555–579.
- Thorman, R. M.; Unlu, I.; Johnson, K. R.; Björnsson, R., McElwee-White, L.; Fairbrother, H.; Ingólfsson, O. (2018) Low energy electron-induced decomposition of (η⁵-Cp)Fe(CO)₂Mn(CO)₅, a potential bimetallic precursor for focused electron beam induced deposition of alloy structures. *Phys. Chem. Chem. Phys.*, *20*, 5644-5656.
- Abbehausen, C.; Ferraz de Paiva, R. E.; Björnsson, R., Quintana Gomes, S.; Du, Z.; Corbi, P. P.; Lima, F. A.; Farrell, N. (2018) X-ray Absorption Spectroscopy Combined with Time-Dependent Density Functional Theory Elucidates Differential Substitution Pathways of Au(I) and Au(III) with Zinc Fingers. *Inorg. Chem.*, *57*, 218-230.

2017

- Benediktsson, B.; Björnsson, R. (2017) QM/MM Study of the Nitrogenase MoFe Protein Resting State: Broken-Symmetry States, Protonation States, and QM Region Convergence in the FeMoco Active Site. *Inorg. Chem.*, *56*, 13417-13429. Free e-print Link
- Ómarsson, B.; Björnsson, R., Ingólfsson, O. (2017) Proton Shuttling and Reactions Paths in Dissociative Electron Attachment to Ortho- and Para-Tetrafluorohydroquinone, an Experimental and Theoretical Study. *J. Phys. Chem. A*, *121*, 5580-5585.
- Kumar T. P., R.; Björnsson, R., Barth, S.; Ingólfsson, O. (2017) Formation and decay of negative ion states up to 11 eV above the ionization energy of the nanofabrication precursor HFeCo₃(CO)₁₂. *Chem. Sci.*, *8*, 5949-5952. Hot article for June!
- Rees, J. A.; Björnsson, R.; Kowalska, J. K.; Lima, F. A.; Schlesier, J.; Sippel, D.; Weyhermüller, T.; Einsle, O.; Kovacs, J. A.; DeBeer, S. (31) Comparative Electronic Structures of Nitrogenase FeMoco and FeVco. *Dalton Trans.*, *46*, 2445-2455.

- Bjornsson, R.; Neese, F.; DeBeer, S. (2017) Revisiting the Mössbauer isomer shifts of the FeMoco cluster of nitrogenase and the cofactor charge. *Inorg. Chem.*, *56*, 1470-1477.
- Belyakov, A. V.; Sigolaev, Y. F.; Shlykov, S. A.; Wallevik, S. Ó.; Jonsdottir, N.R.; Jonsdottir, S.; Kvaran, Á.; Bjornsson, R.; Arnason, I. (2017) Conformational properties of 1-cyano-1-silacyclohexane, C₅H₁₀SiHCN: gas electron diffraction, low-temperature NMR and quantum chemical calculations. *J. Mol. Struct.*, *1132*, 149-156.

2016

- Sigurdardóttir, B. K.; Kvaran, A.; Bjornsson, R.; Arnason, I. (2016) Dissociative Photoionization of 1-Halogenated Silacyclohexanes: Silicon Traps the Halogen. *J. Phys. Chem A.*, *120*, 9188-9197.
- Ólafsson, S. N.; Bjornsson, R.; Helgason, Ö.; Jonsdottir, S.; Suman, S. G. (2016) Coordination geometry determination of stannane compounds with phosphinoyldithioformate ligands using multinuclear NMR, Sn Mössbauer and DFT methods. *J. Organomet. Chem.*, *825-826*, 125-138.
- Thorman, R. M.; Bjornsson, R.; Ingólfsson, O. (2016) Computational study of dissociative electron attachment to π-allyl ruthenium (II) tricarbonyl bromide. *Eur. Phys. J. D*, *70*, 164.
- Kumar T P, R.; Barth, S.; Bjornsson, R.; Ingólfsson, O. (2016) Structure and energetics in dissociative electron attachment to HFeCo₃(CO)₁₂. *Eur. Phys. J. D*, *70*, 163.
- Kowalska, J. K.; Hahn, A. W.; Albers, A.; Schiewer, C. E.; Bjornsson, R.; Lima, F. A.; Meyer, F.; DeBeer, S. (2016) X-ray Absorption and Emission Spectroscopic Studies of [L₂Fe₂S₂]_n Model Complexes: Implications for the Experimental Evaluation of Redox States in Iron–Sulfur Clusters. *Inorg. Chem.*, *55*, 4485-4497.

2015

- Rees, J. A.; Bjornsson, R.; Schlesier, J.; Sippel, D.; Einsle, O.; DeBeer, S. (2015) The Fe-V Cofactor of Vanadium Nitrogenase Contains an Interstitial Carbon. *Atom Angew. Chem. Int. Edit.*, *54*, 13249-13252.
- Bjornsson, R.; Neese, F.; Schrock, R. R.; Einsle, O.; DeBeer, S. (2015) The discovery of Mo(III) in FeMoco: reuniting enzyme and model chemistry. *J. Biol. Inorg. Chem.*, *20*, 447-460. (invited review article)
- Bjornsson, R.; Delgado, M.; Lima, F. A.; Einsle, O.; Neese, F.; DeBeer, S. (2015) Molybdenum L-edges of molybdenum-dependent nitrogenase. *ZAAC*, *641*, 65-71.
- Masters, S.; Robertson, H.; Wann, D.; Hölbling, M.; Hassler, K.; Bjornsson, R.; Wallevik, S. Ó.; Arnason, I. (2015) Molecular Structure of 1,2-bis(trifluoromethyl)-1,1,2,2-tetramethyldisilane in the Gas, Liquid and Solid Phases – Unusual Conformational Changes Between Phases. *J. Phys. Chem. A*, *119*, 1600-1618.
- Belyakov, V.; Sigolaev, Y.; Shlykov, S. A.; Wallevik, S. Ó.; Jonsdottir, N. R.; Bjornsson, R.; Jonsdottir, S.; Kvaran, Á.; Kern, T.; Hassler, K.; Arnason, I. (2015) Conformational properties of 1-tert-butyl-1-silacyclohexane, C₅H₁₀SiH(t-Bu): gas-phase electron diffraction, temperature-dependent Raman spectroscopy and quantum chemical calculations. *Struct Chem.*, *26*, 445-453.

2014

- Cormanich, R. A.; Durie, A.; Bjornsson, R.; Rittner, R.; O'Hagan, D.; Bühl, M. (2014) Density Functional Study of Interactions between Fluorinated Cyclohexanes and Arenes. *Helvetica Chimica Acta*, **97**, 797-807.
- Bjornsson, R.; Lima, F. A.; Weyhermüller, T.; Spatzal, T.; Einsle, O.; Bill, E.; Neese F.; DeBeer, S. (2014) Identification of a spin-coupled Mo(III) in the Nitrogenase Iron-Molybdenum Cofactor. *Chemical Science*, **5**, 3096-3103.

2013

- Lima, F. A.; Bjornsson, R.; Weyhermüller, T.; Chandrasekaran, P.; Glatzel, P.; Neese F.; DeBeer, S. (2013) High-Resolution Molybdenum K-edge X-ray Absorption Spectroscopy analyzed with Time-Dependent Density Functional Theory. *Phys. Chem. Chem. Phys.*, **15**, 20911-20920.
- Wallevik, S. Ó.; Bjornsson, R.; Kvaran, Á.; Jonsdottir, S.; Arnason, I.; Belyakov, A. V.; Baskakov, A. A.; Kern T.; Hassler, K. (2013) Conformational Properties of Halogenated-1-Silacyclohexanes, C₅H₁₀SiHX (X = Cl, Br, I): Gas Electron Diffraction, Low-Temperature NMR, Temperature-Dependent Raman Spectroscopy, and Quantum Chemical Calculations. *Organometallics*, **32**, 6996-7005.
- Jonsdottir, N. R.; Kvaran, Á.; Jonsdottir, S.; Arnason, I.; Bjornsson, R., (2013) Conformational Properties of 1-Methyl-1-Germacyclohexane: Low-Temperature NMR and Quantum Chemical Calculations. *Struct. Chem.*, **2013**, *24*, 769-774.
- Bjornsson, R.; Bühl, M. (2013) Electric field gradients of transition metal complexes: Basis set uncontraction and scalar relativistic effects. *Chem. Phys. Lett.*, **559**, 112-116.

2012

- Kern, T.; Hölbling, M.; Dzambaski, A.; Flock, M.; Hassler, K.; Wallevik, S. Ó.; Arnason I.; Bjornsson, R. (2012) Conformational Energies of Silacyclohexanes C₅H₁₀SiHMe, C₅H₁₀SiH(CF₃) and C₅H₁₀SiCl(SiCl₃) from Variable Temperature Raman Spectra. *J. Raman Spect.*, **43**, 1337-1342.
- Bjornsson R.; Bühl, M. (2012) Modelling Molecular Crystals by QM/MM: Self-Consistent Electrostatic Embedding for Geometry Optimizations and Molecular Property Calculations in the Solid. *J. Chem. Theory Comput.*, **8**, 498-508.
- Cao, J.; Bjornsson, R.; Bühl, M.; Thiel W.; van Mourik T. (2012) Modelling zwitterions in solution: 3-fluoro-γ-aminobutyric acid (3F-GABA). *Chem. Eur. J.*, **18**, 184-195.
- Tacke, R.; Bertermann, R.; Burschka, C.; Dörrich, S.; Fischer, M.; Müller, B.; Meyerhans, G.; Schepmann, D.; Wunsch, B.; Arnason I.; Bjornsson, R. (2012) High-Affinity, Selective Sigma Ligands of the 1,2,3,4-Tetrahydro-1,4'-silaspiro[naphthalene-1,4'-piperidine] Type: Syntheses, Structures, and Pharmacological Properties. *Chem. Med. Chem.*, **7**, 523-532.

2011

- Arnason, I.; Gudnason, P. I.; Bjornsson, R.; Oberhammer, H. (2011) Gas Phase Structures, Energetics, and Potential Energy Surfaces of Disilacyclohexanes. *J. Phys. Chem. A*, **115**, 10000-10008.
- Bjornsson, R.; Früchtl, H.; Bühl, M. (2011) ⁵¹V NMR parameters of VOCl₃: Static and dynamic density functional study from the gas phase to the bulk. *Phys. Chem. Chem. Phys.*, **13**, 619-627.

2010

- Hagan, R. M.; Bjornsson, R.; McMahon, S. A.; Schomburg, B.; Braithwaite, V.; Bühl, M.; Naismith J. H.; Schwarz-Linek, U. (2010) NMR and Theoretical Analysis of a Spontaneously Formed Lys-Asp Isopeptide Bond. *Angew. Chem. Int. Ed.*, **45**, 8421-8425.
- Bjornsson R.; Bühl, M. (2010) Electric Field Gradients of Transition Metal Complexes from Density Functional Theory: Assessment of Functionals, Geometries and Basis sets. *Dalton. T.*, **39**, 5319-5324.
- Wallevik, S. O.; Bjornsson, R.; Kvaran, A.; Jonsdottir, S.; Girichev, G. V.; Giricheva, N. I.; Hassler K.; Arnason, I. (2010) Conformational properties of 1-fluoro-1-methyl-silacyclohexane and 1-methyl-1-trifluoromethyl-1-silacyclohexane: GED, NMR, Raman, and QC calculations. *J. Mol. Struct.*, 209-219.
- Bodi, A.; Bjornsson R.; Arnason I. (2010) A phenomenological relationship between molecular geometry change and conformational energy change. *J. Mol. Struct.* **2010**, *978*, 14-19.
- Wallevik, S. O.; Bjornsson, R.; Kvaran, A.; Jonsdottir, S.; Arnason, I.; Belyakov, A. V.; Baskakov, A. A.; Hassler K.; Oberhammer, H. (2010) Conformational Properties of 1-Silyl-1-Silacyclohexane, C₅H₁₀SiHSiH₃: GED, NMR, Raman, and QC Calculations. *J. Phys. Chem. A*, **114**, 2127-2135.

2009

- Bjornsson, R.; Arnason, I. (2009) Conformational properties of six-membered heterocycles: accurate relative energy differences with DFT, the importance of dispersion interactions and silicon substitution effects. *Phys. Chem. Chem. Phys.*, **11**, 8689-8697.