Ragnar Bjornsson

List of Publications by Year in Descending Order

58 papers	1,347 citations	21 h-index	35 g-index
61 ext. papers	1,618 ext. citations	5.7 avg, IF	4.99 L-index

#	Paper	IF	Citations
58	Carbon Monoxide Binding to the Iron-Molybdenum Cofactor of Nitrogenase: a Detailed Quantum Mechanics/Molecular Mechanics Investigation. *Inorganic Chemistry*, **2021**, 60, 18031-18047	5.1	2
57	Nudged Elastic Band Method for Molecular Reactions Using Energy-Weighted Springs Combined with Eigenvector Following. *Journal of Chemical Theory and Computation*, **2021**, 17, 4929-4945	6.4	22
56	Relative cross sections and appearance energies in electron impact ionization and dissociation of mono-halogenated biphenyls. *International Journal of Mass Spectrometry*, **2021**, 459, 116452	1.9	1
55	Localized and Delocalized States of a Diamine Cation: Resolution of a Controversy. *Journal of Physical Chemistry Letters*, **2021**, 12, 1250-1255	6.4	1
54	The E state of FeMoco: Hydride Formation versus Fe Reduction and a Mechanism for H Evolution. *Chemistry - A European Journal*, **2021**, 27, 16788-16800	4.8	3
53	Caught in the H : Crystal Structure and Spectroscopy Reveal a Sulfur Bound to the Active Site of an O -stable State of [FeFe] Hydrogenase. *Angewandte Chemie - International Edition*, **2020**, 59, 16786-16794	16.4	23
52	Kristallstruktur und Spektroskopie offenbaren einen Schwefel-Liganden am aktiven Zentrum einer O2-stabilen [FeFe]-Hydrogenase. *Angewandte Chemie*, **2020**, 132, 16930	3.6	
51	Insensitivity of Magnetic Coupling to Ligand Substitution in a Series of Tetraoxolene Radical-Bridged Fe Complexes. *Inorganic Chemistry*, **2020**, 59, 4634-4649	5.1	10
50	The Spectroscopy of Nitrogenases. *Chemical Reviews*, **2020**, 120, 5005-5081	68.1	65
49	Dissociation of the FEBID precursor cis-Pt(CO)Cl driven by low-energy electrons. *Physical Chemistry Chemical Physics*, **2020**, 22, 6100-6108	3.6	7
48	Quantum Mechanics/Molecular Mechanics Study of Resting-State Vanadium Nitrogenase: Molecular and Electronic Structure of the Iron-Vanadium Cofactor. *Inorganic Chemistry*, **2020**, 59, 11514-11527	5.1	9
47	Scaffold diversity for enhanced activity of glycosylated inhibitors of fungal adhesion. *RSC Medicinal Chemistry*, **2020**, 11, 1386-1401	3.5	2
46	Resolving the structure of the E state of Mo nitrogenase through Mo and Fe K-edge EXAFS and QM/MM calculations. *Chemical Science*, **2019**, 10, 9807-9821	9.4	19
45	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. *Physical Chemistry Chemical Physics*, **2019**, 21, 4556-4567	3.6	4
44	A model for dinitrogen binding in the E state of nitrogenase. *Chemical Science*, **2019**, 10, 11110-11124	9.4	21
43	Computational Mechanistic Study of [MoFeS] Cubanes for Catalytic Reduction of Nitrogenase Substrates. *Inorganic Chemistry*, **2019**, 58, 1886-1894	5.1	11
42	Multistep Explicit Solvation Protocol for Calculation of Redox Potentials. *Journal of Chemical Theory and Computation*, **2019**, 15, 52-67	6.4	24

41	Low energy electron-induced decomposition of (η5-Cp)Fe(CO)Mn(CO), a potential bimetallic precursor for focused electron beam induced deposition of alloy structures. *Physical Chemistry Chemical Physics*, **2018**, 20, 5644-5656	3.6	8
40	X-ray Absorption Spectroscopy Combined with Time-Dependent Density Functional Theory Elucidates Differential Substitution Pathways of Au(I) and Au(III) with Zinc Fingers. *Inorganic Chemistry*, **2018**, 57, 218-230	5.1	17
39	Electron interactions with the heteronuclear carbonyl precursor HFeRu(CO) and comparison with HFeCo(CO): from fundamental gas phase and surface science studies to focused electron beam induced deposition. *Beilstein Journal of Nanotechnology*, **2018**, 9, 555-579	3	12
38	QM/MM calculations reveal a bridging hydroxo group in a vanadium nitrogenase crystal structure. *Chemical Communications*, **2018**, 54, 7310-7313	5.8	36
37	Revisiting the Mössbauer Isomer Shifts of the FeMoco Cluster of Nitrogenase and the Cofactor Charge. *Inorganic Chemistry*, **2017**, 56, 1470-1477	5.1	79
36	Comparative electronic structures of nitrogenase FeMoco and FeVco. *Dalton Transactions*, **2017**, 46, 2445-2455	4.3	53
35	Formation and decay of negative ion states up to 11 eV above the ionization energy of the nanofabrication precursor HFeCo(CO). *Chemical Science*, **2017**, 8, 5949-5952	9.4	16
34	QM/MM Study of the Nitrogenase MoFe Protein Resting State: Broken-Symmetry States, Protonation States, and QM Region Convergence in the FeMoco Active Site. *Inorganic Chemistry*, **2017**, 56, 13417-13429	5.1	51
33	A combined experimental and theoretical study on dissociative ionization and dissociative electron attachment to the heteronuclear FEBID precursor; HFeCo3(CO)12. *Journal of Physics: Conference Series*, **2017**, 875, 062040	0.3	
32	Proton Shuttling and Reaction Paths in Dissociative Electron Attachment to o- and p-Tetrafluorohydroquinone, an Experimental and Theoretical Study. *Journal of Physical Chemistry A*, **2017**, 121, 5580-5585	2.8	0
31	Conformational properties of 1-cyano-1-silacyclohexane, C5H10SiHCN: Gas electron diffraction, low-temperature NMR and quantum chemical calculations. *Journal of Molecular Structure*, **2017**, 1132, 149-156	3.4	10
30	Coordination geometry determination of stannane compounds with phosphinoyldithioformate ligands using multinuclear NMR, Sn Mössbauer and DFT methods. *Journal of Organometallic Chemistry*, **2016**, 825-826, 125-138	2.3	7
29	Dissociative Photoionization of 1-Halogenated Silacyclohexanes: Silicon Traps the Halogen. *Journal of Physical Chemistry A*, **2016**, 120, 9188-9197	2.8	6
28	Computational study of dissociative electron attachment to η3-allyl ruthenium (II) tricarbonyl bromide. *European Physical Journal D*, **2016**, 70, 1	1.3	7
27	X-ray Absorption and Emission Spectroscopic Studies of [L2Fe2S2](n) Model Complexes: Implications for the Experimental Evaluation of Redox States in Iron-Sulfur Clusters. *Inorganic Chemistry*, **2016**, 55, 4485-97	5.1	53
26	Structure and energetics in dissociative electron attachment to HFeCo3(CO)12. *European Physical Journal D*, **2016**, 70, 1	1.3	15
25	Molybdenum L-Edge XAS Spectra of MoFe Nitrogenase. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2015**, 641, 65-71	1.3	30
24	Molecular structure of 1,2-bis(trifluoromethyl)-1,1,2,2-tetramethyldisilane in the gas, liquid, and solid phases: unusual conformational changes between phases. *Journal of Physical Chemistry A*, **2015**, 119, 1600-8	2.8	2

23	Conformational properties of 1-tert-butyl-1-silacyclohexane, C5H10SiH(t-Bu): gas-phase electron diffraction, temperature-dependent Raman spectroscopy, and quantum chemical calculations. *Structural Chemistry*, **2015**, 26, 445-453	1.8	11
22	The Fe^{V} Cofactor of Vanadium Nitrogenase Contains an Interstitial Carbon Atom. *Angewandte Chemie*, **2015**, 127, 13447-13450	3.6	8
21	The Fe-V Cofactor of Vanadium Nitrogenase Contains an Interstitial Carbon Atom. *Angewandte Chemie - International Edition*, **2015**, 54, 13249-52	16.4	62
20	The discovery of Mo(III) in FeMoco: reuniting enzyme and model chemistry. *Journal of Biological Inorganic Chemistry*, **2015**, 20, 447-60	3.7	63
19	Identification of a spin-coupled Mo(III) in the nitrogenase iron–molybdenum cofactor. *Chemical Science*, **2014**, 5, 3096-3103	9.4	131
18	Density Functional Study of Interactions between Fluorinated Cyclohexanes and Arenes. *Helvetica Chimica Acta*, **2014**, 97, 797-807	2	4
17	High-resolution molybdenum K-edge X-ray absorption spectroscopy analyzed with time-dependent density functional theory. *Physical Chemistry Chemical Physics*, **2013**, 15, 20911-20	3.6	58
16	Conformational properties of 1-methyl-1-germacyclohexane: low-temperature NMR and quantum chemical calculations. *Structural Chemistry*, **2013**, 24, 769-774	1.8	5
15	Electric field gradients of transition metal complexes: Basis set uncontraction and scalar relativistic effects. *Chemical Physics Letters*, **2013**, 559, 112-116	2.5	2
14	Conformational Properties of 1-Halogenated-1-Silacyclohexanes, CHSiHX (X = Cl, Br, I): Gas Electron Diffraction, Low-Temperature NMR, Temperature-Dependent Raman Spectroscopy, and Quantum-Chemical Calculations. *Organometallics*, **2013**, 32, 6996-7005	3.8	24
13	Modelling zwitterions in solution: 3-fluoro-γ-aminobutyric acid (3F-GABA). *Chemistry - A European Journal*, **2012**, 18, 184-95	4.8	11
12	Modeling Molecular Crystals by QM/MM: Self-Consistent Electrostatic Embedding for Geometry Optimizations and Molecular Property Calculations in the Solid. *Journal of Chemical Theory and Computation*, **2012**, 8, 498-508	6.4	32
11	Conformational energies of silacyclohexanes C5H10SiHMe, C5H10SiH(CF3) and C5H10SiCl(SiCl3) from variable temperature Raman spectra. *Journal of Raman Spectroscopy*, **2012**, 43, 1337-1342	2.3	18
10	High-affinity, selective σ ligands of the 1,2,3,4-tetrahydro-1,4Rsilaspiro[naphthalene-1,4Rpiperidine] type: syntheses, structures, and pharmacological properties. *ChemMedChem*, **2012**, 7, 523-32	3.7	19
9	Gas phase structures, energetics, and potential energy surfaces of disilacyclohexanes. *Journal of Physical Chemistry A*, **2011**, 115, 10000-8	2.8	11
8	(51)V NMR parameters of VOCl(3): static and dynamic density functional study from the gas phase to the bulk. *Physical Chemistry Chemical Physics*, **2011**, 13, 619-27	3.6	16
7	Electric field gradients of transition metal complexes from density functional theory: assessment of functionals, geometries and basis sets. *Dalton Transactions*, **2010**, 39, 5319-24	4.3	19
6	Conformational properties of 1-silyl-1-silacyclohexane, C(5)H(10)SiHSiH(3): gas electron diffraction, low-temperature NMR, temperature-dependent Raman spectroscopy, and quantum chemical calculations (&). *Journal of Physical Chemistry A*, **2010**, 114, 2127-35	2.8	38

5	NMR Spectroscopic and Theoretical Analysis of a Spontaneously Formed Lys-Asp Isopeptide Bond. *Angewandte Chemie*, **2010**, 122, 8599-8603	3.6	7
4	NMR spectroscopic and theoretical analysis of a spontaneously formed Lys-Asp isopeptide bond. *Angewandte Chemie - International Edition*, **2010**, 49, 8421-5	16.4	70
3	A phenomenological relationship between molecular geometry change and conformational energy change. *Journal of Molecular Structure*, **2010**, 978, 14-19	3.4	24
2	Conformational properties of 1-fluoro-1-methyl-silacyclohexane and 1-methyl-1-trifluoromethyl-1-silacyclohexane: Gas electron diffraction, low-temperature NMR, temperature-dependent Raman spectroscopy, and quantum chemical calculations. *Journal of Molecular Structure*, **2010**, 978, 209-219	3.4	31
1	Conformational properties of six-membered heterocycles: accurate relative energy differences with DFT, the importance of dispersion interactions and silicon substitution effects. *Physical Chemistry Chemical Physics*, **2009**, 11, 8689-97	3.6	53