Martin Kaupp

List of Publications by Year in Descending Order

385 papers	15,051 citations	64 h-index	97 g-index
416 ext. papers	16,569 ext. citations	7.1 avg, IF	6.8 L-index

#	Paper	IF	Citations
385	Investigation of Molecular Iridium Fluorides IrF (n=1-6): A Combined Matrix-Isolation and Quantum-Chemical Study.. *Chemistry - A European Journal*, **2022**, e202104005	4.8	
384	Extended Benchmark Set of Main-Group Nuclear Shielding Constants and NMR Chemical Shifts and Its Use to Evaluate Modern DFT Methods. *Journal of Chemical Theory and Computation*, **2021**,	6.4	6
383	Competition for Hydride between Silicon and Boron: Synthesis and Characterization of a Hydroborane-Stabilized Silylium Ion.. *Chemistry - A European Journal*, **2021**, e202104464	4.8	0
382	Local hybrid functionals augmented by a strong-correlation model. *Journal of Chemical Physics*, **2021**, 155, 144101	3.9	0
381	The Supramolecular Structural Chemistry of Pentafluorosulfanyl and Tetrafluorosulfanylene Compounds. *Chemistry - A European Journal*, **2021**, 27, 6086-6093	4.8	3
380	Implementation and Validation of Local Hybrid Functionals with Calibrated Exchange-Energy Densities for Nuclear Shielding Constants. *Journal of Physical Chemistry A*, **2021**, 125, 2697-2707	2.8	3
379	Tetryl-Tetrylene Addition to Phenylacetylene. *Chemistry - A European Journal*, **2021**, 27, 4691-4699	4.8	2
378	Iron Versus Ruthenium: Evidence for the Distinct Differences in the Electronic Structures of Hexa-1,3,5-triyn-1,6-diyl-bridged Complexes [Cp*(dppe)M}{Ł(C?C)3}{M(dppe)Cp*}]+ (M = Fe, Ru). *Organometallics*, **2021**, 40, 346-357	3.8	1
377	Effect of the Current Dependence of Tau-Dependent Exchange-Correlation Functionals on Nuclear Shielding Calculations. *Journal of Chemical Theory and Computation*, **2021**, 17, 1469-1479	6.4	7
376	Reliable TDDFT Protocol Based on a Local Hybrid Functional for the Prediction of Vibronic Phosphorescence Spectra Applied to Tris(2,2'-bipyridine)-Metal Complexes. *Journal of Physical Chemistry A*, **2021**, 125, 7099-7110	2.8	4
375	Matrix Isolation Spectroscopic and Relativistic Quantum Chemical Study of Molecular Platinum Fluorides PtF (n=1-6) Reveals Magnetic Bistability of PtF. *Chemistry - A European Journal*, **2021**, 27, 13642-13650	4.8	3
374	Assessment of hybrid functionals for singlet and triplet excitations: Why do some local hybrid functionals perform so well for triplet excitation energies?. *Journal of Chemical Physics*, **2021**, 155, 124108	3.9	3
373	Platinum Indolylphosphine Fluorido and Polyfluorido Complexes: An Interplay between Cyclometallation, Fluoride Migration, and Hydrogen Bonding. *Chemistry - A European Journal*, **2021**, 27, 14287-14298	4.8	2
372	Novel synthetic pathway for the production of phosgene. *Science Advances*, **2021**, 7, eabj5186	14.3	1
371	ReSpect: Relativistic spectroscopy DFT program package. *Journal of Chemical Physics*, **2020**, 152, 184101	3.9	41
370	Verbesserter Zugang zu organisch lŁslichen Di- und Tetrafluoridochlorat(I/III)-Salzen. *Angewandte Chemie*, **2020**, 132, 16136-16140	3.6	4
369	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. *Journal of Chemical Physics*, **2020**, 152, 184107	3.9	255

368	Improved Access to Organo-Soluble Di- and Tetrafluoridochlorate(I)/(III) Salts. *Angewandte Chemie - International Edition*, **2020**, 59, 16002-16006	16.4	7
367	Relativistic Heavy-Neighbor-Atom Effects on NMR Shifts: Concepts and Trends Across the Periodic Table. *Chemical Reviews*, **2020**, 120, 7065-7103	68.1	47
366	Covalent vs Charge-Shift Nature of the Metal-Metal Bond in Transition Metal Complexes: A Unified Understanding. *Journal of the American Chemical Society*, **2020**, 142, 12277-12287	16.4	19
365	A four-parameter system for rationalising the electronic properties of transition metal-radical ligand complexes. *Dalton Transactions*, **2020**, 49, 9735-9742	4.3	4
364	C vs C Bond Cleavage of Triphenylphosphine at Platinum(0): Mechanism of Formation, Reactivity, Redox Chemistry, and NMR Chemical Shift Calculations of a Phosphanido Diplatinum(II) Platform. *Organometallics*, **2020**, 39, 443-452	3.8	5
363	An Efficient Coupled-Perturbed Kohn-Sham Implementation of NMR Chemical Shift Computations with Local Hybrid Functionals and Gauge-Including Atomic Orbitals. *Journal of Chemical Theory and Computation*, **2020**, 16, 931-943	6.4	19
362	Noncollinear Relativistic Two-Component X2C Calculations of Hyperfine Couplings Using Local Hybrid Functionals. Importance of the High-Density Coordinate Scaling Limit. *Journal of Chemical Theory and Computation*, **2020**, 16, 314-325	6.4	11
361	Electronic States of 2,3-Diamino-1,4-naphthoquinone and Its N-Alkylated Derivatives. *Journal of Physical Chemistry C*, **2020**, 124, 60-69	3.8	7
360	Nuclear Spin-Spin Couplings: Efficient Evaluation of Exact Exchange and Extension to Local Hybrid Functionals. *Journal of Physical Chemistry A*, **2020**, 124, 8529-8539	2.8	10
359	A Local Hybrid Functional with Wide Applicability and Good Balance between (De)Localization and Left-Right Correlation. *Journal of Chemical Theory and Computation*, **2020**, 16, 5645-5657	6.4	18
358	Validation of Local Hybrid Functionals for Excited States: Structures, Fluorescence, Phosphorescence, and Vibronic Spectra. *Journal of Chemical Theory and Computation*, **2020**, 16, 5821-5834	6.4	9
357	Hyperfine-Coupling Tensors from Projected Hartree-Fock Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 6222-6235	6.4	1
356	Evaluation of an Efficient 3D-RISM-SCF Implementation as a Tool for Computational Spectroscopy in Solution. *Journal of Physical Chemistry A*, **2020**, 124, 7439-7452	2.8	6
355	Picometer Resolution Structure of the Coordination Sphere in the Metal-Binding Site in a Metalloprotein by NMR. *Journal of the American Chemical Society*, **2020**, 142, 16757-16765	16.4	19
354	Evaluation of Local Hybrid Functionals for Electric Properties: Dipole Moments and Static and Dynamic Polarizabilities. *Journal of Physical Chemistry A*, **2020**, 124, 8346-8358	2.8	6
353	Stable Actinide Complexes of a Neutral 1,4-Diborabenzene. *Angewandte Chemie - International Edition*, **2020**, 59, 13109-13115	16.4	7
352	Hydroxy-bridged resting states of a [NiFe]-hydrogenase unraveled by cryogenic vibrational spectroscopy and DFT computations. *Chemical Science*, **2020**, 12, 2189-2197	9.4	7
351	Development and Implementation of Excited-State Gradients for Local Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2019**, 15, 5508-5522	6.4	12

350	Asymmetry in the Ligand Coordination Sphere of the [FeFe] Hydrogenase Active Site Is Reflected in the Magnetic Spin Interactions of the Aza-propanedithiolate Ligand. *Journal of Physical Chemistry Letters*, **2019**, 10, 6794-6799	6.4	13
349	Density Functional Calculations of Electron Paramagnetic Resonance g- and Hyperfine-Coupling Tensors Using the Exact Two-Component (X2C) Transformation and Efficient Approximations to the Two-Electron Spin-Orbit Terms. *Journal of Physical Chemistry A*, **2019**, 123, 5660-5672	2.8	11
348	C□H and C□F Bond Activation Reactions of Fluorinated Propenes at Rhodium: Distinctive Reactivity of the Refrigerant HFO-1234yf. *Angewandte Chemie*, **2019**, 131, 10798-10802	3.6	7
347	Quantum-chemical study of Li NMR shifts in the context of delithiation of paramagnetic lithium vanadium phosphate, LiV(PO) (LVP). *Solid State Nuclear Magnetic Resonance*, **2019**, 101, 89-100	3.1	2
346	C-H and C-F Bond Activation Reactions of Fluorinated Propenes at Rhodium: Distinctive Reactivity of the Refrigerant HFO-1234yf. *Angewandte Chemie - International Edition*, **2019**, 58, 10688-10692	16.4	13
345	A Spectroscopic and Computationally Minimal Approach to the Analysis of Charge-Transfer Processes in Conformationally Fluxional Mixed-Valence and Heterobimetallic Complexes. *Chemistry - A European Journal*, **2019**, 25, 8837-8853	4.8	12
344	A Silylene-Borane Lewis Pair as a Tool for Trapping a Water Molecule: Silanol Formation and Dehydrogenation. *Chemistry - A European Journal*, **2019**, 25, 4678-4682	4.8	7
343	Computation of NMR Shifts for Paramagnetic Solids Including Zero-Field-Splitting and Beyond-DFT Approaches. Application to LiMPO4(M = Mn, Fe, Co, Ni) and MPO4(M = Fe, Co). *Journal of Physical Chemistry C*, **2019**, 123, 8387-8405	3.8	13
342	Local hybrid functionals: Theory, implementation, and performance of an emerging new tool in quantum chemistry and beyond. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1378	7.9	60
341	Insights from Te and Fe nuclear resonance vibrational spectroscopy: a [4Fe-4Te] cluster from two points of view. *Chemical Science*, **2019**, 10, 7535-7541	9.4	2
340	Characterization of hydrogen-substituted silylium ions in the condensed phase. *Science*, **2019**, 365, 168-172	33.3	23
339	Hubbard Trimer with Spin-Orbit Coupling: Hartree-Fock Solutions, (Non)Collinearity, and Anisotropic Spin Hamiltonian. *Journal of Physical Chemistry A*, **2019**, 123, 2361-2378	2.8	3
338	Activation of tetrafluoropropenes by rhodium(i) germyl and silyl complexes. *Faraday Discussions*, **2019**, 220, 328-349	3.6	4
337	Ligand Effects on the Reactivity of [CoX]+ (X = CN, F, Cl, Br, O, OH) Towards CO2: Gas-Phase Generation of the Elusive Cyanoformate by [Co(CN)]+ and [Fe(CN)]+. *Topics in Catalysis*, **2018**, 61, 575-584	2.3	7
336	Quantum-Chemical Approach to NMR Chemical Shifts in Paramagnetic Solids Applied to LiFePO and LiCoPO. *Journal of Physical Chemistry Letters*, **2018**, 9, 1480-1484	6.4	20
335	Noncollinear Two-Component Quasirelativistic Description of Spin Interactions in Exchange-Coupled Systems. Mapping Generalized Broken-Symmetry States to Effective Spin Hamiltonians. *Journal of Chemical Theory and Computation*, **2018**, 14, 1267-1276	6.4	2
334	Exact Mapping from Many-Spin Hamiltonians to Giant-Spin Hamiltonians. *Chemistry - A European Journal*, **2018**, 24, 4689-4702	4.8	5
333	Probing Interactions of N-Donor Molecules with Open Metal Sites within Paramagnetic Cr-MIL-101: A Solid-State NMR Spectroscopic and Density Functional Theory Study. *Journal of the American Chemical Society*, **2018**, 140, 2135-2144	16.4	32

332	Iron versus Ruthenium: Clarifying the Electronic Differences between Prototypical Mixed-Valence Organometallic Butadiyndiyl Bridged Molecular Wires. *Organometallics*, **2018**, 37, 1432-1445	3.8	33
331	MVO-10: A Gas-Phase Oxide Benchmark for Localization/Delocalization in Mixed-Valence Systems. *Journal of Chemical Theory and Computation*, **2018**, 14, 3512-3523	6.4	12
330	Large-Scale Computation of Nuclear Magnetic Resonance Shifts for Paramagnetic Solids Using CP2K. *Journal of Chemical Theory and Computation*, **2018**, 14, 377-394	6.4	25
329	Lessons from the Spin-Polarization/Spin-Contamination Dilemma of Transition-Metal Hyperfine Couplings for the Construction of Exchange-Correlation Functionals. *Journal of Chemical Theory and Computation*, **2018**, 14, 5653-5672	6.4	22
328	Innenr□ktitelbild: An Isolable Silicon Dicarbonate Complex from Carbon Dioxide Activation with a Silylone (Angew. Chem. 7/2017). *Angewandte Chemie*, **2017**, 129, 1957-1957	3.6	
327	An Isolable Silicon Dicarbonate Complex from Carbon Dioxide Activation with a Silylone. *Angewandte Chemie*, **2017**, 129, 1920-1923	3.6	19
326	An Isolable Silicon Dicarbonate Complex from Carbon Dioxide Activation with a Silylone. *Angewandte Chemie - International Edition*, **2017**, 56, 1894-1897	16.4	37
325	Internal Dynamics of the 3-Pyrroline-N-Oxide Ring in Spin-Labeled Proteins. *Journal of Physical Chemistry Letters*, **2017**, 8, 1113-1117	6.4	1
324	DFT investigation of the effect of spin-orbit coupling on the NMR shifts in paramagnetic solids. *Physical Review B*, **2017**, 95,	3.3	23
323	Chemistry is about energy and its changes: A critique of bond-length/bond-strength correlations. *Coordination Chemistry Reviews*, **2017**, 344, 355-362	23.2	58
322	Taming Silicon Congeners of CO and CO : Synthesis of Monomeric Si and Si Chalcogenide Complexes. *Angewandte Chemie - International Edition*, **2017**, 56, 6298-6301	16.4	20
321	Taming Silicon Congeners of CO and CO2: Synthesis of Monomeric SiII and SiIV Chalcogenide Complexes. *Angewandte Chemie*, **2017**, 129, 6395-6398	3.6	7
320	Metal-Dependent Strengthening and Weakening of M-H and M-C Bonds by an Oxo Ligand: Thermal Gas-Phase Activation of Methane by [OMH] and [MH] (M=Mo, Ti). *Chemistry - A European Journal*, **2017**, 23, 12346-12352	4.8	6
319	Insights into trans-Ligand and Spin-Orbit Effects on Electronic Structure and Ligand NMR Shifts in Transition-Metal Complexes. *Chemistry - A European Journal*, **2017**, 23, 9790-9803	4.8	36
318	Development of a TDDFT-Based Protocol with Local Hybrid Functionals for the Screening of Potential Singlet Fission Chromophores. *Journal of Chemical Theory and Computation*, **2017**, 13, 4984-4996	5.4	43
317	On the Electronic Origin of Remarkable Ligand Effects on the Reactivities of [NiL] Complexes (L=C H , C H N, CN) towards Methane. *Chemistry - A European Journal*, **2017**, 23, 14430-14433	4.8	4
316	Reactivity of the Sterically Demanding Siloxanediol Mes Si(OH)(□O)Si(OH)Mes Towards Water and Ether Molecules. *Chemistry - A European Journal*, **2017**, 23, 13964-13972	4.8	3
315	Insights into trans-Ligand and Spin-Orbit Effects on Electronic Structure and Ligand NMR Shifts in Transition-Metal Complexes. *Chemistry - A European Journal*, **2017**, 23, 9702-9702	4.8	3

314	Four-Component Relativistic Density Functional Calculations of EPR Parameters for Model Complexes of Tungstoenzymes. *Journal of Physical Chemistry A*, **2017**, 121, 9106-9117	2.8	4
313	A high-spin square planar iron(ii)-siloxide and its tetrahedral allogon - structural and spectroscopic models of Fe-zeolite sites. *Chemical Communications*, **2017**, 53, 8081-8084	5.8	11
312	On the Activation of Methane and Carbon Dioxide by [HTaO](+) and [TaOH](+) in the Gas Phase: A Mechanistic Study. *Chemistry - A European Journal*, **2016**, 22, 10581-9	4.8	16
311	[Al2O4](-), a Benchmark Gas-Phase Class II Mixed-Valence Radical Anion for the Evaluation of Quantum-Chemical Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 3796-806	6.4	15
310	Pseudo-Contact NMR Shifts over the Paramagnetic Metalloprotein CoMMP-12 from First Principles. *Angewandte Chemie - International Edition*, **2016**, 55, 14713-14717	16.4	45
309	Giant spin-orbit effects on H and C NMR shifts for uranium(vi) complexes revisited: role of the exchange-correlation response kernel, bonding analyses, and new predictions. *Physical Chemistry Chemical Physics*, **2016**, 18, 30462-30474	3.6	33
308	Tetrakis(ferrocenylethynyl)ethene: Synthesis, (Spectro)electrochemical and quantum chemical characterisation. *Journal of Organometallic Chemistry*, **2016**, 821, 40-47	2.3	11
307	Wavelength selective polymer network formation of end-functional star polymers. *Chemical Communications*, **2016**, 52, 1975-8	5.8	39
306	Gauge effects in local hybrid functionals evaluated for weak interactions and the GMTKN30 test set. *Molecular Physics*, **2016**, 114, 1118-1127	1.7	23
305	The M□sbauer Parameters of the Proximal Cluster of Membrane-Bound Hydrogenase Revisited: A Density Functional Theory Study. *Journal of Chemical Theory and Computation*, **2016**, 12, 174-87	6.4	10
304	Mechanistic aspects of CO2 activation mediated by phenyl yttrium cation: A combined experimental/theoretical study. *Journal of Catalysis*, **2016**, 343, 68-74	7.3	9
303	Construction of Giant-Spin Hamiltonians from Many-Spin Hamiltonians by Third-Order Perturbation Theory and Application to an Fe3 Cr Single-Molecule Magnet. *Chemistry - A European Journal*, **2016**, 22, 6853-62	4.8	5
302	Validation of local hybrid functionals for TDDFT calculations of electronic excitation energies. *Journal of Chemical Physics*, **2016**, 144, 074106	3.9	93
301	New approaches for the calibration of exchange-energy densities in local hybrid functionals. *Physical Chemistry Chemical Physics*, **2016**, 18, 21133-44	3.6	26
300	Electron transfer pathways in mixed-valence paracyclophane-bridged bis-triarylamine radical cations. *Journal of Computational Chemistry*, **2016**, 37, 93-102	3.5	8
299	Completing the Heterocubane Family [Cp*AlE]4 (E = O, S, Se, and Te) by Selective Oxygenation and Sulfuration of [Cp*Al]4: Density Functional Theory Calculations of [Cp*AlE]4 and Reactivity of [Cp*AlO]4 toward Hydrolysis. *Inorganic Chemistry*, **2016**, 55, 4915-23	5.1	33
298	Paramagnetic NMR of Phenolic Oxime Copper Complexes: A Joint Experimental and Density Functional Study. *Chemistry - A European Journal*, **2016**, 22, 15328-15339	4.8	17
297	Implementation of Molecular Gradients for Local Hybrid Density Functionals Using Seminumerical Integration Techniques. *Journal of Chemical Theory and Computation*, **2016**, 12, 4254-62	6.4	23

296	Tracking Transient Conformational States of T4 Lysozyme at Room Temperature Combining X-ray Crystallography and Site-Directed Spin Labeling. *Journal of the American Chemical Society*, **2016**, 138, 12868-12875	16.4	6
295	Understanding Thermodynamic and Spectroscopic Properties of Tetragonal Mn12 Single-Molecule Magnets from Combined Density Functional Theory/Spin-Hamiltonian Calculations. *Journal of Physical Chemistry A*, **2016**, 120, 6864-79	2.8	13
294	Rational Control of Conformational Distributions and Mixed-Valence Characteristics in Diruthenium Complexes. *Chemistry - A European Journal*, **2016**, 22, 16138-16146	4.8	27
293	A Relativistic Quantum-Chemical Analysis of the trans Influence on (1)H NMR Hydride Shifts in Square-Planar Platinum(II) Complexes. *Inorganic Chemistry*, **2015**, 54, 7199-208	5.1	54
292	Efficient Self-Consistent Implementation of Local Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2015**, 11, 1540-8	6.4	44
291	Relativistic and Solvation Effects on the Stability of Gold(III) Halides in Aqueous Solution. *Inorganic Chemistry*, **2015**, 54, 9869-75	5.1	11
290	Mechanism of the cooperative Si-H bond activation at Ru-S bonds. *Chemical Science*, **2015**, 6, 4324-4334	9.4	69
289	Controlled ligand distortion and its consequences for structure, symmetry, conformation and spin-state preferences of iron(II) complexes. *Dalton Transactions*, **2015**, 44, 19232-47	4.3	12
288	Cross-Conjugated Systems Based On An (E)-Hexa-3-en-1,5-diyne-3,4-diyl Skeleton: Spectroscopic and Spectroelectrochemical Investigations. *Journal of Organic Chemistry*, **2015**, 80, 11501-12	4.2	6
287	Correlations between metal spin states and vibrational spectra of a trinuclear Fe(II) complex exhibiting spin crossover. *Journal of Molecular Structure*, **2015**, 1101, 8-13	3.4	2
286	Efficient Semi-numerical Implementation of Global and Local Hybrid Functionals for Time-Dependent Density Functional Theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 4226-37	6.4	39
285	Validation of the direct-COSMO-RS solvent model for Diels-Alder reactions in aqueous solution. *Journal of Chemical Theory and Computation*, **2015**, 11, 111-21	6.4	12
284	Synthesis and redox properties of mono-, di- and tri-metallic platinum-ethynyl complexes based on the trans-Pt(C6H4N{C6H4OCH3-4}2)(C CR)(PPh3)2 motif. *Polyhedron*, **2015**, 86, 31-42	2.7	5
283	Design of exchange-correlation functionals through the correlation factor approach. *Journal of Chemical Physics*, **2015**, 143, 144102	3.9	25
282	Biomimetic [2Fe-2S] clusters with extensively delocalized mixed-valence iron centers. *Angewandte Chemie - International Edition*, **2015**, 54, 12506-10	16.4	25
281	From Silylone to an Isolable Monomeric Silicon Disulfide Complex. *Angewandte Chemie*, **2015**, 127, 10392-10395	2.0	15
280	From Silylone to an Isolable Monomeric Silicon Disulfide Complex. *Angewandte Chemie - International Edition*, **2015**, 54, 10254-7	16.4	41
279	Four-Component Relativistic Density Functional Theory Calculations of EPR g- and Hyperfine-Coupling Tensors Using Hybrid Functionals: Validation on Transition-Metal Complexes with Large Tensor Anisotropies and Higher-Order Spin-Orbit Effects. *Journal of Physical Chemistry A* , **2015**, 119, 12892-905	2.8	38

278	On ammonia binding to the oxygen-evolving complex of photosystem II: a quantum chemical study. *Chemistry - A European Journal*, **2014**, 20, 7300-8	4.8	29
277	Reversible [4Fe-3S] cluster morphing in an O(2)-tolerant [NiFe] hydrogenase. *Nature Chemical Biology*, **2014**, 10, 378-85	11.7	70
276	Ligand spheres in asymmetric hetero Diels-Alder reactions catalyzed by Cu(II) box complexes: experiment and modeling. *Dalton Transactions*, **2014**, 43, 698-705	4.3	10
275	Quantum-chemical insights into mixed-valence systems: within and beyond the Robin-Day scheme. *Chemical Society Reviews*, **2014**, 43, 5067-88	58.5	132
274	Synthesis and vibrational spectroscopy of (57)Fe-labeled models of [NiFe] hydrogenase: first direct observation of a nickel-iron interaction. *Chemical Communications*, **2014**, 50, 13469-72	5.8	12
273	A combined computational and spectroelectrochemical study of platinum-bridged bis-triarylamine systems. *Inorganic Chemistry*, **2014**, 53, 1544-54	5.1	37
272	Combined Spectroscopic and Quantum Chemical Study of [trans-Ru(C?CC6H4R1-4)2(dppe)2]n+ and [trans-Ru(C?CC6H4R1-4)(C?CC6H4R2-4)(dppe)2]n+ (n = 0, 1) Complexes: Interpretations beyond the Lowest Energy Conformer Paradigm. *Organometallics*, **2014**, 33, 4947-4963	3.8	58
271	Synthesis, Reactivity, and Electronic Structure of a Bioinspired Heterobimetallic [Ni(□S2)Fe] Complex with Disulfur Monoradical character. *Organometallics*, **2014**, 33, 3154-3162	3.8	3
270	Mixed-valence ruthenium complexes rotating through a conformational Robin-Day continuum. *Chemistry - A European Journal*, **2014**, 20, 6895-908	4.8	59
269	Insight into the mechanism of carbonyl hydrosilylation catalyzed by Brookhart's cationic iridium(III) pincer complex. *Journal of the American Chemical Society*, **2014**, 136, 6912-5	16.4	81
268	Chemical Bonding of Main-Group Elements **2014**, 1-24		8
267	Towards improved local hybrid functionals by calibration of exchange-energy densities. *Journal of Chemical Physics*, **2014**, 141, 204101	3.9	49
266	Communication: A non-empirical correlation factor model for the exchange-correlation energy. *Journal of Chemical Physics*, **2014**, 141, 111102	3.9	30
265	Redox-dependent structural transformations of the [4Fe-3S] proximal cluster in O2-tolerant membrane-bound [NiFe]-hydrogenase: a DFT study. *Journal of the American Chemical Society*, **2013**, 135, 11809-23	16.4	25
264	Understanding Structure Formation in Organolithium Compounds: An Experimental and Quantum-Chemical Approach. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2013**, 639, 2077-2085	1.3	19
263	From bis(silylene) and bis(germylene) pincer-type nickel(II) complexes to isolable intermediates of the nickel-catalyzed Sonogashira cross-coupling reaction. *Journal of the American Chemical Society*, **2013**, 135, 15617-26	16.4	189
262	A heterobimetallic approach to stabilize the elusive disulfur radical trianion ("subsulfide") S2(□-). *Chemistry - A European Journal*, **2013**, 19, 1246-53	4.8	9
261	Ab Initio and Density Functional Calculations of Electronic g-Tensors for Organic Radicals. *Progress in Theoretical Chemistry and Physics*, **2013**, 323-361	0.6	

260	The preparation, characterisation and electronic structures of 2,4-pentadiynylnitrile (cyanobutadiynyl) complexes. *Dalton Transactions*, **2013**, 42, 4240-3	4.3	6
259	Syntheses, Spectroelectrochemical Studies, and Molecular and Electronic Structures of Ferrocenyl Ene-diynes. *Organometallics*, **2013**, 32, 6022-6032	3.8	20
258	A rare uranyl(VI)-alkyl ate complex [Li(DME)1.5]2[UO2(CH2SiMe3)4] and its comparison with a homoleptic uranium(VI)-hexaalkyl. *Angewandte Chemie - International Edition*, **2013**, 52, 3259-63	16.4	59
257	Refining the interpretation of near-infrared band shapes in a polyynediyl molecular wire. *Chemistry - A European Journal*, **2013**, 19, 9780-4	4.8	51
256	A Rare Uranyl(VI)Alkyl Ate Complex [Li(DME)1.5]2[UO2(CH2SiMe3)4] and Its Comparison with a Homoleptic Uranium(VI)Hexaalkyl. *Angewandte Chemie*, **2013**, 125, 3341-3345	3.6	13
255	The family of ferrocene-stabilized silylium ions: synthesis, 29Si NMR characterization, Lewis acidity, substituent scrambling, and quantum-chemical analyses. *Chemistry - A European Journal*, **2013**, 19, 16579-94	4.8	67
254	Synthesis and bonding in carbene complexes of an unsymmetrical dilithio methandiide: a combined experimental and theoretical study. *Chemistry - A European Journal*, **2013**, 19, 16729-39	4.8	62
253	Reliable Quantum Chemical Prediction of the Localized/Delocalized Character of Organic Mixed-Valence Radical Anions. From Continuum Solvent Models to Direct-COSMO-RS. *Journal of Chemical Theory and Computation*, **2012**, 8, 4189-203	6.4	70
252	Gigantische Spin-Bahn-Effekte auf NMR-Verschiebungen in diamagnetischen Actinoid-Komplexen: Richtlinien fdie Suche nach Uran(VI)-Hydridkomplexen. *Angewandte Chemie*, **2012**, 124, 11042-11046	3.6	11
251	Giant spin-orbit effects on NMR shifts in diamagnetic actinide complexes: guiding the search of uranium(VI) hydride complexes in the correct spectral range. *Angewandte Chemie - International Edition*, **2012**, 51, 10884-8	16.4	73
250	Can zinc really exist in its oxidation state +III?. *Journal of the American Chemical Society*, **2012**, 134, 11977-9	11.4	20
249	Predicting the localized/delocalized character of mixed-valence diquinone radical anions. Toward the right answer for the right reason. *Journal of Physical Chemistry A*, **2012**, 116, 10629-37	2.8	45
248	Synthesis, structure, and reactivity of borole-functionalized ferrocenes. *Chemistry - A European Journal*, **2012**, 18, 11732-46	4.8	37
247	Neutral Metal Atoms Acting as a Leaving Group in Gas-Phase SN2 Reactions: M(CH3)+ + NH3 -h CH3NH3+ + M (M = Zn, Cd, Hg). *Organometallics*, **2012**, 31, 3816-3824	3.8	26
246	A facile route to boronic acid functional polymeric microspheres via epoxide ring opening. *Macromolecular Rapid Communications*, **2012**, 33, 1108-13	4.8	13
245	[TeX3]+ Cations Stabilized by the Weakly Coordinating [Al(ORF)4]Anion: FIR Spectra, Raman Spectra, and Evaluation of an Abnormal Halogen Dependence of the 125Te NMR Chemical Shifts. *ChemPlusChem*, **2012**, 77, 643-651	2.8	13
244	Importance of the correlation contribution for local hybrid functionals: range separation and self-interaction corrections. *Journal of Chemical Physics*, **2012**, 136, 014111	3.9	62
243	Elucidating mechanisms in haem copper oxidases: the high-affinity QH binding site in quinol oxidase as studied by DONUT-HYSCORE spectroscopy and density functional theory. *Faraday Discussions*, **2011**, 148, 315-44; discussion 421-41	3.6	14

242	Nuclear Magnetic Resonance (NMR) Parameters of Transition Metal Complexes: Methods and Applications **2011**,		1
241	Evaluation of a combination of local hybrid functionals with DFT-D3 corrections for the calculation of thermochemical and kinetic data. *Journal of Physical Chemistry A*, **2011**, 115, 8990-6	2.8	25
240	Relativistic four-component DFT calculations of 1H NMR chemical shifts in transition-metal hydride complexes: unusual high-field shifts beyond the Buckingham-Stephens model. *Journal of Physical Chemistry A*, **2011**, 115, 5654-9	2.8	106
239	Structure of the oxygen-rich cluster cation Al2O7+ and its reactivity toward methane and water. *Journal of the American Chemical Society*, **2011**, 133, 16930-7	16.4	69
238	A neutral, monomeric germanium(I) radical. *Journal of the American Chemical Society*, **2011**, 133, 10074-7	16.4	86
237	Computational and spectroscopic studies of organic mixed-valence compounds: where is the charge?. *Physical Chemistry Chemical Physics*, **2011**, 13, 16973-86	3.6	102
236	Assessment of higher-order spin□orbit effects on electronic g-tensors of d 1 transition-metal complexes by relativistic two- and four-component methods. *Theoretical Chemistry Accounts*, **2011**, 129, 715-725	1.9	36
235	Advances in local hybrid exchange-correlation functionals: from thermochemistry to magnetic-resonance parameters and hyperpolarizabilities. *International Journal of Quantum Chemistry*, **2011**, 111, 2625-2638	2.1	40
234	Computation of hyperfine tensors for dinuclear Mn(III) Mn(IV) complexes by broken-symmetry approaches: anisotropy transfer induced by local zero-field splitting. *ChemPhysChem*, **2011**, 12, 3170-9	3.2	24
233	Analysis of tertiary phosphanes, arsanes, and stibanes as bridging ligands in dinuclear Group 9 complexes. *Chemistry - A European Journal*, **2011**, 17, 7228-35	4.8	7
232	Squaraine dyes as efficient coupling bridges between triarylamine redox centres. *Chemistry - A European Journal*, **2011**, 17, 14147-63	4.8	60
231	Cluster or periodic, static or dynamic--the challenge of calculating the g tensor of the solid-state glycine radical. *Physical Chemistry Chemical Physics*, **2011**, 13, 18638-46	3.6	16
230	Impact of molecular flexibility on binding strength and self-sorting of chiral □surfaces. *Journal of the American Chemical Society*, **2011**, 133, 9580-91	16.4	87
229	From silicon(II)-based dioxygen activation to adducts of elusive dioxasiliranes and sila-ureas stable at room temperature. *Nature Chemistry*, **2010**, 2, 577-80	17.6	128
228	The □-Furfuryl Ligand: Plausible Catalytic Intermediates and Heterocyclic □-Benzyl Analogues with Superior Binding Ability. *Organometallics*, **2010**, 29, 4431-4433	3.8	10
227	Phosphorus chemical shifts in a nucleic acid backbone from combined molecular dynamics and density functional calculations. *Journal of the American Chemical Society*, **2010**, 132, 17139-48	16.4	38
226	Activation of ammonia by a Si=O double bond and formation of a unique pair of sila-hemiaminal and silanoic amide tautomers. *Journal of the American Chemical Society*, **2010**, 132, 6912-3	16.4	102
225	Hyperfine coupling constants of the nitrogen and phosphorus atoms: A challenge for exact-exchange density-functional and post-Hartree□Fock methods. *Journal of Chemical Physics*, **2010**, 132, 184107	3.9	14

224	On Occupied-orbital Dependent Exchange-correlation Functionals: From Local Hybrids to Becke B05 Model. *Zeitschrift Fur Physikalische Chemie*, **2010**, 224, 545-567	3.1	8
223	Modeling environmental effects on charge density distributions in polar organometallics: validation of embedded cluster models for the methyl lithium crystal. *Journal of Computational Chemistry*, **2010**, 31, 2568-76	3.5	11
222	Electronic structure and reactivity of a [1],[1]disilamolybdenocenophane. *Chemistry - A European Journal*, **2010**, 16, 3014-20	4.8	10
221	Neutral penta- and hexacoordinate silicon(IV) complexes containing two bidentate ligands derived from the alpha-amino acids (S)-alanine, (S)-phenylalanine, and (S)-tert-leucine. *Chemistry - A European Journal*, **2010**, 16, 6582-9	4.8	26
220	Density functional calculations of (55)Mn, (14)N and (13)C electron paramagnetic resonance parameters support an energetically feasible model system for the S(2) state of the oxygen-evolving complex of photosystem II. *Chemistry - A European Journal*, **2010**, 16, 10424-38	4.8	68
219	On Occupied-orbital Dependent Exchange-correlation Functionals: From Local Hybrids to Beckes B05 Model **2010**, 255-277		1
218	On the self-consistent implementation of general occupied-orbital dependent exchange-correlation functionals with application to the B05 functional. *Journal of Chemical Physics* , **2009**, 131, 084103	3.9	24
217	Comparative analysis of electron-density and electron-localization function for dinuclear manganese complexes with bridging boron- and carbon-centered ligands. *Chemistry - A European Journal*, **2009**, 15, 623-32	4.8	36
216	Synthesis, structure, and bonding of novel homodinuclear cobalt and nickel borylene complexes. *Chemistry - A European Journal*, **2009**, 15, 7150-5	4.8	10
215	Silicon analogues of the RXR-selective retinoid agonist SR11237 (BMS649): chemistry and biology. *ChemMedChem*, **2009**, 4, 1143-52	3.7	36
214	Formation and Characterization of the Iridium Tetroxide Molecule with Iridium in the Oxidation State +VIII. *Angewandte Chemie*, **2009**, 121, 8019-8023	3.6	23
213	Ein dreikerniger Boridkomplex mit einer fluktuierenden Gold-Bor-Bindung. *Angewandte Chemie*, **2009**, 121, 9916-9919	3.6	25
212	Formation and characterization of the iridium tetroxide molecule with iridium in the oxidation state +VIII. *Angewandte Chemie - International Edition*, **2009**, 48, 7879-83	16.4	56
211	A trimetallic gold boride complex with a fluxional gold-boron bond. *Angewandte Chemie - International Edition*, **2009**, 48, 9735-8	16.4	51
210	Relativistic two-component calculations of electronic g-tensor for oxo-molybdenum(V) and oxo-tungsten(V) complexes: The important role of higher-order spin-orbit contributions. *Chemical Physics*, **2009**, 356, 229-235	2.3	20
209	Metal–Metal Distances at the Limit: Cr–Cr 1.73 Å, the Importance of the Ligand and its Fine Tuning. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2009**, 635, 1149-1152	1.3	98
208	Carboalumination of a chromium–chromium quintuple bond. *Nature Chemistry*, **2009**, 1, 322-5	17.6	119
207	The highest oxidation states of the transition metal elements. *Coordination Chemistry Reviews*, **2009**, 253, 606-624	23.2	145

206	Combining NMR spectroscopy and quantum chemistry as tools to quantify spin density distributions in molecular magnetic compounds. *Coordination Chemistry Reviews*, **2009**, 253, 2376-2386	23.2	93
205	Diphosphines with strongly polarized P-P bonds: hybrids between covalent molecules and donor-acceptor adducts with flexible molecular structures. *Journal of the American Chemical Society* , **2009**, 131, 10763-74	16.4	39
204	Jacobsen's catalyst for hydrolytic kinetic resolution: structure elucidation of paramagnetic Co(III) salen complexes in solution via combined NMR and quantum chemical studies. *Journal of the American Chemical Society*, **2009**, 131, 4172-3	16.4	50
203	Coupled-Perturbed Scheme for the Calculation of Electronic g-Tensors with Local Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2009**, 5, 2985-95	6.4	15
202	Understanding ground- and excited-state properties of perylene tetracarboxylic acid bisimide crystals by means of quantum chemical computations. *Journal of the American Chemical Society*, **2009**, 131, 15660-8	16.4	94
201	Local hybrid functionals with an explicit dependence on spin polarization. *Journal of Physical Chemistry A*, **2009**, 113, 11898-906	2.8	41
200	Characteristic spin-orbit induced 1H(CH2) chemical shifts upon deprotonation of group 9 polyamine aqua and alcohol complexes. *Journal of the American Chemical Society*, **2009**, 131, 11909-18	16.4	24
199	Disila-Phantolide and Derivatives: Synthesis and Olfactory Characterization of Silicon-Containing Derivatives of the Musk Odorant Phantolide. *Organometallics*, **2009**, 28, 4700-4712	3.8	28
198	Validation of broken-symmetry density functional methods for the calculation of electron paramagnetic resonance parameters of dinuclear mixed-valence MnIVMnIII complexes. *Canadian Journal of Chemistry*, **2009**, 87, 1521-1539	0.9	32
197	A reliable quantum-chemical protocol for the characterization of organic mixed-valence compounds. *Journal of the American Chemical Society*, **2009**, 131, 16292-302	16.4	154
196	Density functional theory study of the oxoperoxo vanadium(V) complexes of glycolic acid. Structural correlations with NMR chemical shifts. *Dalton Transactions*, **2009**, 9735-45	4.3	28
195	Structure of the nucleotide radical formed during reaction of CDP/TTP with the E441Q-alpha2beta2 of E. coli ribonucleotide reductase. *Journal of the American Chemical Society*, **2009**, 131, 200-11	16.4	50
194	Quantum chemical study of trivalent group 12 fluorides. *Inorganic Chemistry*, **2008**, 47, 3379-83	5.1	28
193	Oxoperoxo vanadium(V) complexes of L-lactic acid: density functional theory study of structure and NMR chemical shifts. *Inorganic Chemistry*, **2008**, 47, 7317-26	5.1	25
192	Exciton trapping in pi-conjugated materials: a quantum-chemistry-based protocol applied to perylene bisimide dye aggregates. *Journal of the American Chemical Society*, **2008**, 130, 12858-9	16.4	258
191	Synthesis, Crystal Structure, EPR and DFT Studies, and Redox Properties of [2]Tetramethyldisilacobaltocenophane. *Organometallics*, **2008**, 27, 6427-6433	3.8	30
190	Synthesis, reactivity, and electronic structure of [n]vanadoarenophanes: an experimental and theoretical study. *Journal of the American Chemical Society*, **2008**, 130, 11376-93	16.4	51
189	Stable CI3+ salts and attempts to prepare CHI2+ and CH2I+. *Dalton Transactions*, **2008**, 946-56	4.3	27

188	Synthesis and structure of a ferrocenylboron dication. *Inorganic Chemistry*, **2008**, 47, 7456-8	5.1	34
187	A fully relativistic method for calculation of nuclear magnetic shielding tensors with a restricted magnetically balanced basis in the framework of the matrix Dirac-Kohn-Sham equation. *Journal of Chemical Physics*, **2008**, 128, 104101	3.9	169
186	What can we learn from the adiabatic connection formalism about local hybrid functionals?. *Journal of Chemical Physics*, **2008**, 128, 214107	3.9	43
185	Car-Parrinello molecular dynamics simulations and EPR property calculations on aqueous ubisemiquinone radical anion. *Theoretical Chemistry Accounts*, **2008**, 119, 477-487	1.9	26
184	Structure and electron paramagnetic resonance parameters of the manganese site of concanavalin A studied by density functional methods. *Theoretical Chemistry Accounts*, **2008**, 120, 437-445	1.9	7
183	Is Allred's [Hg(cyclam)]3+ a true mercury(III) complex?. *Angewandte Chemie - International Edition*, **2008**, 47, 8631-3	16.4	17
182	Is Allred's [Hg(cyclam)]3+ a True Mercury(III) Complex?. *Angewandte Chemie*, **2008**, 120, 8759-8761	3.6	8
181	Computational studies of electron paramagnetic resonance parameters for paramagnetic molybdenum complexes. 1. Method validation on small and medium-sized systems. *Journal of Physical Chemistry B*, **2007**, 111, 4616-29	3.4	30
180	Computational studies of EPR parameters for paramagnetic molybdenum complexes. II. Larger MoV systems relevant to molybdenum enzymes. *Inorganic Chemistry*, **2007**, 46, 8146-61	5.1	25
179	High-valent technetium fluorides. Does TcF7 exist?. *Inorganic Chemistry*, **2007**, 46, 5734-8	5.1	14
178	Density functional study of EPR parameters and spin-density distribution of azurin and other blue copper proteins. *Journal of Physical Chemistry B*, **2007**, 111, 8290-304	3.4	59
177	Understanding the electon paramagnetic resonance parameters of protein-bound glycyl radicals. *Journal of Physical Chemistry B*, **2007**, 111, 820-31	3.4	10
176	Understanding the EPR parameters of glycine-derived radicals: the case of N-acetylglycyl in the N-acetylglycine single-crystal environment. *Journal of Physical Chemistry B*, **2007**, 111, 811-9	3.4	16
175	Local hybrid functionals: an assessment for thermochemical kinetics. *Journal of Chemical Physics*, **2007**, 127, 194102	3.9	75
174	Unusual silicon coordination polyhedra: non-VSEPR structures of zwitterionic lambda5-Si silicon(IV) complexes with an SiS2N2C or SiS2O2C skeleton. *Angewandte Chemie - International Edition*, **2007**, 46, 7001-5	16.4	25
173	Mercury is a transition metal: the first experimental evidence for HgF(4). *Angewandte Chemie - International Edition*, **2007**, 46, 8371-5	16.4	103
172	Unusual Silicon Coordination Polyhedra: Non-VSEPR Structures of Zwitterionic λ5-Si Silicon(IV) Complexes with an SiS2N2C or SiS2O2C Skeleton. *Angewandte Chemie*, **2007**, 119, 7131-7135	3.6	18
171	Mercury Is a Transition Metal: The First Experimental Evidence for HgF4. *Angewandte Chemie*, **2007**, 119, 8523-8527	3.6	43

170	The role of radial nodes of atomic orbitals for chemical bonding and the periodic table. *Journal of Computational Chemistry*, **2007**, 28, 320-5	3.5	84
169	Hyperfine coupling tensors of the benzosemiquinone radical anion from Car-Parrinello molecular dynamics. *ChemPhysChem*, **2007**, 8, 69-79	3.2	23
168	Local hybrid exchange-correlation functionals based on the dimensionless density gradient. *Chemical Physics Letters*, **2007**, 440, 160-168	2.5	90
167	Nuclear shielding constants from localized local hybrid exchange-correlation potentials. *Chemical Physics Letters*, **2007**, 442, 496-503	2.5	24
166	The New Si-Silicate Dianion [Si(NCO)6]2Synthesis and Structural Characterization of [K(18-crown-6)]2[Si(NCO)6]. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2007**, 633, 2667-2670	1.3	14
165	A thermochemically competitive local hybrid functional without gradient corrections. *Journal of Chemical Physics*, **2007**, 126, 011103	3.9	101
164	Density functional calculations of NMR shielding tensors for paramagnetic systems with arbitrary spin multiplicity: validation on 3d metallocenes. *Journal of Chemical Physics*, **2007**, 126, 024107	3.9	85
163	Revising the highest oxidation states of the 5d elements: the case of iridium(+VII). *Angewandte Chemie - International Edition*, **2006**, 45, 3708-11	16.4	31
162	Die höchsten Oxidationszustände der 5d-Elemente: der Fall Iridium(+VII). *Angewandte Chemie*, **2006**, 118, 3791-3794	3.6	10
161	Resolution of identity Dirac-Kohn-Sham method using the large component only: Calculations of g-tensor and hyperfine tensor. *Journal of Chemical Physics*, **2006**, 124, 084108	3.9	36
160	From local hybrid functionals to "localized local hybrid" potentials: formalism and thermochemical tests. *Journal of Chemical Physics*, **2006**, 124, 204102	3.9	63
159	Scalar relativistic calculations of hyperfine coupling tensors using the Douglas-Kroll-Hess method with a finite-size nucleus model. *Physical Chemistry Chemical Physics*, **2006**, 8, 4079-85	3.6	48
158	New route to 1-thia-closo-dodecaborane(11), closo-1-SB11H11, and its halogenation reactions. The effect of the halogen on the dipole moments and the NMR spectra and the importance of spin-orbit coupling for the 11B chemical shifts. *Dalton Transactions*, **2006**, 1024-9	4.3	30
157	Has AuF7 been made?. *Inorganic Chemistry*, **2006**, 45, 1228-34	5.1	51
156	Where is the limit of highly fluorinated high-oxidation-state osmium species?. *Inorganic Chemistry*, **2006**, 45, 10497-502	5.1	14
155	Protein-cofactor interactions and EPR parameters for the Q(H) quinone binding site of quinol oxidase. A density functional study. *Journal of the American Chemical Society*, **2006**, 128, 5659-71	16.4	30
154	Molecular mechanical devices based on quinone-pyrrole and quinone-indole dyads: a computational study. *Journal of Physical Chemistry B*, **2006**, 110, 8158-65	3.4	8
153	Density functional study of electron paramagnetic resonance parameters and spin density distributions of dicopper(I) complexes with bridging azo and tetrazine radical-anion ligands. *Journal of Physical Chemistry A*, **2006**, 110, 4021-33	2.8	17

152	Calculation of zero-field splitting parameters: comparison of a two-component noncolinear spin-density-functional method and a one-component perturbational approach. *Journal of Chemical Physics*, **2006**, 125, 054110	3.9	59
151	Normalization of the effective exchange hole in Becke's nondynamical correlation model: Closed-form analytic representation. *Computational and Theoretical Chemistry*, **2006**, 762, 151-158		11
150	Structure of the nitrogen-centered radical formed during inactivation of E. coli ribonucleotide reductase by 2'-azido-2'-deoxyuridine-5'-diphosphate: trapping of the 3'-ketonucleotide. *Journal of the American Chemical Society*, **2005**, 127, 7729-38	16.4	45
149	Comparative density-functional study of the electron paramagnetic resonance parameters of amavadin. *Journal of Physical Chemistry B*, **2005**, 109, 4227-33	3.4	23
148	A Heterotopically Chelated Low-Valent Lead Amide1. *Organometallics*, **2005**, 24, 3576-3578	3.8	27
147	Understanding structure and bonding in early actinide 6d(0)5f0 MX6q (M = Th-Np; X = H, F) complexes in comparison with their transition metal 5d0 analogues. *Journal of the American Chemical Society*, **2005**, 127, 2591-9	16.4	46
146	Understanding Substituent Effects on 29Si Chemical Shifts and Bonding in Disilynes. A Quantum-Chemical Analysis. *Organometallics*, **2005**, 24, 6331-6337	3.8	20
145	Where is the spin? Understanding electronic structure and g-tensors for ruthenium complexes with redox-active quinonoid ligands. *Journal of the American Chemical Society*, **2005**, 127, 11399-413	16.4	148
144	Relativistic two-component calculations of electronic g-tensors that include spin polarization. *Journal of Chemical Physics*, **2005**, 123, 244103	3.9	65
143	Calculation of 19F NMR chemical shifts in uranium complexes using density functional theory and pseudopotentials. *Chemical Physics*, **2005**, 311, 45-56	2.3	35
142	[Pb5{Mo(CO)3}2]4-: a complex containing a planar Pb5 unit. *Angewandte Chemie - International Edition*, **2005**, 44, 2092-6	16.4	60
141	[Pb5{Mo(CO)3}2]4□ein Polyanion mit einer planaren Pb5-Einheit. *Angewandte Chemie*, **2005**, 117, 2129-2133	3.6	11
140	Extended Car-Parrinello molecular dynamics and electronic g-tensors study of benzosemiquinone radical anion. *Magnetic Resonance in Chemistry*, **2005**, 43 Spec no., S237-47	2.1	29
139	Understanding the conformational dependence of spin-spin coupling constants: through-bond and through-space J(31P,31P) coupling in tetraphosphane-1,4-diides [M(L)x]2[P4R4]. *Chemistry - A European Journal*, **2005**, 11, 2773-82	4.8	29
138	Can weakly coordinating anions stabilize mercury in its oxidation state +IV?. *Chemistry - A European Journal*, **2005**, 11, 2743-55	4.8	34
137	Understanding solvent effects on hyperfine coupling constants of cyclohexadienyl radicals. *Theoretical Chemistry Accounts*, **2005**, 114, 318-326	1.9	11
136	Localized hybrid exchange-correlation potentials for Kohn□Sham DFT calculations of NMR and EPR parameters. *International Journal of Quantum Chemistry*, **2005**, 104, 261-271	2.1	29
135	Use of Continuum Solvent Models in Magnetic Resonance Parameter Calculations **2004**, 191-208		11

134	Ro-Vibrational Corrections to NMR Parameters **2004**, 153-173		53
133	Interpretation of NMR Chemical Shifts **2004**, 293-306		25
132	Relativistic Calculations of Spin–Spin Coupling Constants of Heavy Nuclei **2004**, 249-264		30
131	Perturbational and ECP Calculation of Relativistic Effects in NMR Shielding and Spin–Spin Coupling **2004**, 209-226		47
130	Calculations of Magnetic Resonance Parameters in Solids and Liquids Using Periodic Boundary Conditions **2004**, 265-277		3
129	Chemical Shifts with Hartree–Fock and Density Functional Methods **2004**, 83-100		3
128	Calculation of Heavy-Nucleus Chemical Shifts. Relativistic All-Electron Methods **2004**, 227-247		34
127	Calculation of EPR g-Tensors with Density Functional Theory **2004**, 505-532		20
126	First-Principles Calculations of Paramagnetic NMR Shifts **2004**, 325-338		40
125	Theory of NMR Parameters. From Ramsey to Relativity, 1953 to 1983 **2004**, 7-19		6
124	Electron-Correlated Methods for the Calculation of NMR Chemical Shifts **2004**, 123-139		23
123	Ab Initio Post-Hartree–Fock Calculations of Hyperfine Coupling Tensors and Their Comparison with DFT Approaches **2004**, 483-492		5
122	Molecular Dynamics and NMR Parameter Calculations **2004**, 175-189		11
121	Relativistic spin-orbit effects on hyperfine coupling tensors by density-functional theory. *Journal of Chemical Physics*, **2004**, 120, 2127-39	3.9	83
120	The Effective Spin Hamiltonian Concept from a Quantum Chemical Perspective **2004**, 33-41		1
119	Solvent effects on g-tensors of semiquinone radical anions: polarizable continuum versus cluster models. *Theoretical Chemistry Accounts*, **2004**, 111, 132-140	1.9	42
118	Trigonal prismatic or not trigonal prismatic? On the mechanisms of oxygen-atom transfer in molybdopterin-based enzymes. *Angewandte Chemie - International Edition*, **2004**, 43, 546-9	16.4	29
117	On the lack of correlation between bond lengths, dissociation energies, and force constants: the fluorine-substituted ethane homologues. *Inorganica Chimica Acta*, **2004**, 357, 1865-1872	2.7	29

116	Construction of local hybrid exchange-correlation potentials and their evaluation for nuclear shielding constants. *Chemical Physics Letters*, **2004**, 386, 8-16	2.5	41
115	Unrestricted open-shell Kohn Sham scheme with local hybrid exchange-correlation potentials: improved calculation of electronic g-tensors for transition-metal complexes. *Chemical Physics Letters*, **2004**, 391, 16-21	2.5	33
114	Scalar relativistic calculations of hyperfine coupling tensors using the Douglas Kroll Hess method. *Chemical Physics Letters*, **2004**, 396, 268-276	2.5	52
113	Validation of density functional methods for computing structures and energies of mercury(IV) complexes. *Physical Chemistry Chemical Physics*, **2004**, 6, 1122	3.6	53
112	Spin Orbit Effects on Hyperfine Coupling Tensors in Transition Metal Complexes Using Hybrid Density Functionals and Accurate Spin Orbit Operators. *Journal of Physical Chemistry A*, **2004**, 108, 5026-5033	2.8	59
111	Electronic g-Tensors of Semiquinones in Photosynthetic Reaction Centers. A Density Functional Study. *Journal of Physical Chemistry B*, **2004**, 108, 2464-2469	3.4	26
110	Introduction: The Quantum Chemical Calculation of NMR and EPR Parameters **2004**, 1-5		1
109	DFT Calculations of EPR Hyperfine Coupling Tensors **2004**, 461-482		9
108	Alternative Fermi Contact Operators for EPR and NMR **2004**, 493-504		1
107	Zero-Field Splitting **2004**, 541-564		19
106	Computation of Hyperfine Coupling Tensors to Complement EPR Experiments **2004**, 565-580		
105	Ab Initio Calculations of g-Tensors **2004**, 533-540		1
104	Aromaticity Indices from Magnetic Shieldings **2004**, 395-407		8
103	Calculation of Nuclear Quadrupole Coupling Constants **2004**, 279-291		32
102	Characterizing Two-Bond NMR 13C?15N, 15N?15N, and 19F?15N Spin Spin Coupling Constants across Hydrogen Bonds Using Ab Initio EOM-CCSD Calculations **2004**, 353-370		8
101	Calculation of NMR Parameters in Carbocation Chemistry **2004**, 371-394		2
100	Interpretation of Indirect Nuclear Spin Spin Coupling Constants **2004**, 307-324		5
99	Unexpected 29Si NMR Chemical Shifts in Heteroatom-Substituted Silyllithium Compounds: A Quantum-Chemical Analysis. *Organometallics*, **2004**, 23, 3647-3655	3.8	38

98	Spin-orbit-induced anomalous pH-dependence in (1)H NMR spectra of Co(III) amine complexes: a diagnostic tool for structure elucidation. *Journal of the American Chemical Society*, **2004**, 126, 6728-38	16.4	22
97	Ab initio molecular dynamics simulations and g-tensor calculations of aqueous benzosemiquinone radical anion: effects of regular and "T-stacked" hydrogen bonds. *Journal of the American Chemical Society*, **2004**, 126, 9854-61	16.4	53
96	Semiempirical Methods for the Calculation of NMR Chemical Shifts **2004**, 141-152		1
95	13C NMR study of halogen bonding of haloarenes: measurements of solvent effects and theoretical analysis. *Journal of the American Chemical Society*, **2004**, 126, 4412-9	16.4	115
94	Relativistic Effects on NMR Chemical Shifts. *Theoretical and Computational Chemistry*, **2004**, 14, 552-597		47
93	Spin□Spin Coupling Constants with HF and DFT Methods **2004**, 101-121		22
92	NMR Parameters in Proteins and Nucleic Acids **2004**, 339-351		1
91	NMR of Transition Metal Compounds **2004**, 421-431		22
90	Applications to EPR in Bioinorganic Chemistry **2004**, 581-591		7
89	Historical Aspects of EPR Parameter Calculations **2004**, 21-32		15
88	Fundamentals of Nonrelativistic and Relativistic Theory of NMR and EPR Parameters **2004**, 43-82		10
87	Fullerenes **2004**, 409-420		0
86	Characterization of NMR Tensors via Experiment and Theory **2004**, 433-447		11
85	Calculations of Nuclear Magnetic Resonance Parameters in Zeolites **2004**, 449-460		0
84	The self-consistent implementation of exchange-correlation functionals depending on the local kinetic energy density. *Chemical Physics Letters*, **2003**, 381, 495-504	2.5	51
83	Elementares Gallium als Quelle f□niedervalente Gallium-Liganden in neuartigen Ga-Rh-Clustern. *Angewandte Chemie*, **2003**, 115, 5237-5240	3.6	1
82	Elemental gallium as a source of subvalent gallium units in gallium-rhodium clusters. *Angewandte Chemie - International Edition*, **2003**, 42, 5083-6	16.4	9
81	Understanding Substituent Effects on 29Si Chemical Shifts and Bonding in Disilenes. A Quantum Chemical Analysis□ *Organometallics*, **2003**, 22, 2442-2449	3.8	55

80	New Zwitterionic Spirocyclic 5Si-Silicates with an SiX4C Skeleton (X = S, O) Containing Two Ligands of the Dithiolato(2) or Diolato(2) Type: Synthesis, Structure, and Bonding Situations. *Organometallics*, **2003**, 22, 4104-4110	3.8	42
79	Reaction of Pentadienyl Complexes with Metal Carbonyls: Synthetic, Structural, and Theoretical Studies of Metallabenzene Complexes. *Organometallics*, **2003**, 22, 264-274	3.8	40
78	gTensor and Spin Density of the Modified Tyrosyl Radical in Galactose Oxidase: A Density Functional Study. *Journal of Physical Chemistry B*, **2003**, 107, 331-337	3.4	38
77	In Situ Study on the Wet Chemical Synthesis of Nanoscopic Pt Colloids by Reductive Stabilization. *Journal of Physical Chemistry B*, **2003**, 107, 7507-7515	3.4	39
76	AB Initio and Density Functional Calculations of Electronic G-Tensors for Organic Radicals. *Progress in Theoretical Chemistry and Physics*, **2003**, 267-302	0.6	10
75	Calculation of electronic g-tensors for transition metal complexes using hybrid density functionals and atomic meanfield spin-orbit operators. *Journal of Computational Chemistry*, **2002**, 23, 794-803	3.5	166
74	Trigonal Prismatic Structure of Tris(butadiene)molybdenum and Related Complexes Revisited: Diolefin or Metallacyclopentene Coordination?. *Organometallics*, **2002**, 21, 5021-5028	3.8	15
73	The function of photosystem I. Quantum chemical insight into the role of tryptophan-quinone interactions. *Biochemistry*, **2002**, 41, 2895-900	3.2	51
72	Density functional calculations of electronic g-tensors for semiquinone radical anions. The role of hydrogen bonding and substituent effects. *Journal of the American Chemical Society*, **2002**, 124, 2709-22	16.4	89
71	Validation study of meta-GGA functionals and of a model exchange-correlation potential in density functional calculations of EPR parameters. *Physical Chemistry Chemical Physics*, **2002**, 4, 5467-5474	3.6	63
70	Understanding the unusual g-values and the spin density distribution of hydrogen atoms trapped in silasesquioxanes. *Physical Chemistry Chemical Physics*, **2002**, 4, 5458-5466	3.6	14
69	Multifrequency EPR study and density functional g-tensor calculations of persistent organorhenium radical complexes. *Journal of the American Chemical Society*, **2002**, 124, 10563-71	16.4	55
68	Nicht-VSEPR-Strukturen und chemische Bindung in d0-Systemen. *Angewandte Chemie*, **2001**, 113, 3642-3677	3.6	35
67	"Non-VSEPR" Structures and Bonding in d(0) Systems. *Angewandte Chemie - International Edition*, **2001**, 40, 3534-3565	16.4	131
66	A Density Functional Study of EPR Parameters for Vanadyl Complexes Containing Schiff Base Ligands. *Journal of Physical Chemistry B*, **2001**, 105, 12644-12652	3.4	64
65	Study of relativistic effects on nuclear shieldings using density-functional theory and spin-orbit pseudopotentials. *Journal of Chemical Physics*, **2001**, 114, 61	3.9	90
64	Characterisation of the tetrahalophosphonium cations PBrnI4 −n+ (0 ≤ n ≤ 4) by 31P MAS NMR, IR and Raman spectroscopy and the crystal structures of PI4+AlCl4−, PI4+AlBr4− and PI4+GaI4− *Dalton Transactions RSC*, **2001**, 1880-1889		16
63	Zusammenbruch der Korrelation zwischen Bindungslänge und Bindungsstärke – eine Fallstudie. *Angewandte Chemie*, **2000**, 112, 4780-4782	3.6	35

62	Breakdown of Bond Length-Bond Strength Correlation: A Case Study. *Angewandte Chemie - International Edition*, **2000**, 39, 4607-4609	16.4	92
61	Density Functional Calculations of Electronic g-Tensors Using Spin□Orbit Pseudopotentials and Mean-Field All-Electron Spin□Orbit Operators. *Journal of the American Chemical Society*, **2000**, 122, 9206-9218	16.4	211
60	Mechanisms of EPR Hyperfine Coupling in Transition Metal Complexes. *Journal of the American Chemical Society*, **2000**, 122, 11900-11913	16.4	132
59	Density Functional Study of 17O NMR Chemical Shift and Nuclear Quadrupole Coupling Tensors in Oxyheme Model Complexes. *Journal of Physical Chemistry B*, **2000**, 104, 5200-5208	3.4	22
58	The PI4+ cation has an extremely large negative 31P nuclear magnetic resonance chemical shift, due to spin□orbit coupling: A quantum-chemical prediction and its confirmation by solid-state nuclear magnetic resonance spectroscopy. *Journal of Chemical Physics*, **1999**, 110, 3897-3902	3.9	40
57	The DFT route to NMR chemical shifts. *Journal of Computational Chemistry*, **1999**, 20, 91-105	3.5	245
56	The role of □-type nonbonding orbitals for spin□orbit induced NMR chemical shifts: DFT study of 13C and 19F shifts in the series CF3IFn (n=0, 2, 4, 6). *Journal of Computational Chemistry*, **1999**, 20, 1304-1313	3.5	35
55	The [Sn5]2□Cluster Compound [K-(2,2,2-crypt)]2Sn5 □Synthesis, Crystal Structure, Raman Spectrum, and Hierarchical Relationship to CaIn2. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **1999**, 625, 37-42	1.3	21
54	Im Niemandsland der Sechsfach-Koordination bei d0-□bergangsmetallkomplexen: Strukturvorhersagen f□ [WCl5CH3], [WCl4(CH3)2] und [WCl3(CH3)3]. *Angewandte Chemie*, **1999**, 111, 3219-3221	3.6	6
53	The Coordination Chemistry of the CF Group of Fluorocarbons: Thermodynamic Data and Ab Initio Calculations on CF□Metal Ion Interactions. *Chemistry - A European Journal*, **1999**, 5, 2566-2572	4.8	24
52	On the Relation between □Bonding, Electronegativity, and Bond Angles in High-Valent Transition Metal Complexes. *Chemistry - A European Journal*, **1999**, 5, 3631-3643	4.8	39
51	Charting No-Man's Land in d(0) Transition Metal Six-Coordination: Structure Predictions for the Complexes. *Angewandte Chemie - International Edition*, **1999**, 38, 3034-3037	16.4	6
50	A Critical Validation of Density Functional and Coupled-Cluster Approaches for the Calculation of EPR Hyperfine Coupling Constants in Transition Metal Complexes. *Journal of Physical Chemistry A*, **1999**, 103, 9966-9983	2.8	251
49	Spin□orbit corrections to NMR shielding constants from density functional theory. How important are the two-electron terms?. *Chemical Physics Letters*, **1998**, 296, 93-104	2.5	102
48	Das Clusteranion Si94□*Angewandte Chemie*, **1998**, 110, 2507-2509	3.6	30
47	How Do Spin□Orbit-Induced Heavy-Atom Effects on NMR Chemical Shifts Function? Validation of a Simple Analogy to Spin□Spin Coupling by Density Functional Theory (DFT) Calculations on Some Iodo Compounds. *Chemistry - A European Journal*, **1998**, 4, 118-126	4.8	305
46	The Nonoctahedral Structures of d0, d1, and d2 Hexamethyl Complexes. *Chemistry - A European Journal*, **1998**, 4, 1678-1686	4.8	45
45	The Unusual Fluxional Structure of Tetramethyloxotungsten: Quantum Chemical Structure Predictions for the d0 and d1 Complexes [MOR4] (M=W, Re; R=H, CH3). *Chemistry - A European Journal*, **1998**, 4, 2059-2071	4.8	9

44	The Cluster Anion Si. *Angewandte Chemie - International Edition*, **1998**, 37, 2359-2361	16.4	46
43	Systematic Experimental and Quantum Chemical Investigation into the Structures, the Stability, and the Spectroscopic Properties of Alkylindium(I) Compounds: Tetrameric In4[C(SiMeRR)3]4 versus Monomeric InC(SiMeRR)3 Derivatives. *Organometallics*, **1998**, 17, 5009-5017	3.8	54
42	Solid-State Nuclear Magnetic Resonance Spectroscopic and Quantum Chemical Investigation of13C and17O Chemical Shift Tensors,17O Nuclear Quadrupole Coupling Tensors, and Bonding in Transition-Metal Carbonyl Complexes and Clusters. *Journal of the American Chemical Society*, **1998**, 120, 4771-4783	16.4	44
41	Density functional analysis of 13C and 1H chemical shifts and bonding in mercurimethanes and organomercury hydrides: The role of scalar relativistic, spin-orbit, and substituent effects. *Journal of Chemical Physics*, **1998**, 108, 3648-3659	3.9	68
40	The calculation of 17O chemical shielding in transition metal oxo complexes. I. Comparison of DFT and ab initio approaches, and mechanisms of relativity-induced shielding. *Journal of Chemical Physics*, **1997**, 106, 9201-9212	3.9	68
39	Theoretische Chemie 1996. *Nachrichten Aus Der Chemie*, **1997**, 45, 180-187		1
38	Sn6(PR)6], [Sn3(Pr)2, and [Cu24(PR)12] (R = Triorganoisilyl): New Tin and Copper Phosphanediyl Clusters. *Angewandte Chemie International Edition in English*, **1997**, 36, 1894-1896		32
37	Interpretation of 13C NMR chemical shifts in halomethyl cations. On the importance of spin-orbit coupling and electron correlation. *Chemical Physics Letters*, **1997**, 265, 55-59	2.5	83
36	The Structure of Hexamethyltungsten, W(CH3)6: Distorted Trigonal Prismatic with C3 Symmetry. *Journal of the American Chemical Society*, **1996**, 118, 3018-3024	16.4	72
35	The Structure of XeF6 and of Compounds Isoelectronic with It. A Challenge to Computational Chemistry and to the Qualitative Theory of the Chemical Bond. *Journal of the American Chemical Society*, **1996**, 118, 11939-11950	16.4	62
34	13 C NMR chemical-shift tensors of interstitial carbides in transition-metal clusters calculated by density-functional theory. *Chemical Communications*, **1996**, 1141	5.8	21
33	Ab Initio ECP/DFT Calculation and Interpretation of Carbon and Oxygen NMR Chemical Shift Tensors in Transition-Metal Carbonyl Complexes. *Chemistry - A European Journal*, **1996**, 2, 24-30	4.8	47
32	NMR Chemical-Shift Anomaly and Bonding in Piano-Stool Carbonyl and Related Complexes. An Ab Initio ECP/DFT Study. *Chemistry - A European Journal*, **1996**, 2, 348-358	4.8	22
31	Analysis of 13C and 17O Chemical Shift Tensors and an ELF View of Bonding in Fe2(CO)9 and Rh6(CO)16. *Chemische Berichte*, **1996**, 129, 527-533		26
30	Interpretation of 31P-NMR Coordination Shifts for Phosphane Ligands. Ab Initio ECP/DFT Study of Chemical Shift Tensors in M(CO)5L [M = Cr, Mo, W; L = PH3, P(CH3)3, PF3, PCl3]. *Chemische Berichte*, **1996**, 129, 535-544		35
29	Scalar Relativistic Effects on 17O NMR Chemical Shifts in Transition-Metal Oxo Complexes. An ab Initio ECP/DFT Study. *Journal of the American Chemical Society*, **1995**, 117, 1851-1852	16.4	72
28	Scalar Relativistic Effects on 17O NMR Chemical Shifts in Transition-Metal Oxo Complexes. An ab Initio ECP/DFT Study. [Erratum to document cited in CA122:254385]. *Journal of the American Chemical Society*, **1995**, 117, 8492-8492	16.4	17
27	Formale Oxidationsstufe versus Partialladung. Ein Kommentar. *Angewandte Chemie*, **1995**, 107, 1076-1076	3.6	13

26	Formal Oxidation State versus Partial Charge—A Comment. *Angewandte Chemie International Edition in English*, **1995**, 34, 986-986		43
25	Pressure-Induced Phase Transition in CsGeBr3 Studied by X-Ray Diffraction and Raman Spectroscopy. *Journal of Solid State Chemistry*, **1995**, 118, 20-27	3.3	29
24	Calculation of ligand NMR chemical shifts in transition-metal complexes using ab initio effective-core potentials and density functional theory. *Chemical Physics Letters*, **1995**, 235, 382-388	2.5	79
23	Alkylation Reactions of Dialkylzinc Compounds with 1,4-Diaza-1,3-butadienes: Cationic and Radical Anionic Organozinc Intermediates. Molecular Structure of the Cationic Organozinc Species [MeZn(tert-BuN:CHCH:N-tert-Bu)]O3SCF3 and Me2Zn(bpy) (bpy = 2,2'-Bipyridine). *Organometallics*, **1994**, 13, 2349-2356	3.8	34
22	Dominance of Linear 2-Coordination in Mercury Chemistry: Quasirelativistic and Nonrelativistic ab Initio Pseudopotential Study of (HgX2)2 (X = F, Cl, Br, I, H). *Inorganic Chemistry*, **1994**, 33, 2555-2564	5.1	82
21	Oxidation State +IV in Group 12 Chemistry. Ab Initio Study of Zinc(IV), Cadmium(IV), and Mercury(IV) Fluorides. *Inorganic Chemistry*, **1994**, 33, 2122-2131	5.1	72
20	Ab Initio Comparison of the (MX2)2 Dimers (M = Zn, Cd, Hg; X = F, Cl, H) and Study of Relativistic Effects in Crystalline HgF2. *Inorganic Chemistry*, **1994**, 33, 4718-4722	5.1	28
19	Origin of the Unique Stability of Condensed-Phase Hg22+. An ab Initio Investigation of MI and MII Species (M = Zn, Cd, Hg). *Inorganic Chemistry*, **1994**, 33, 4179-4185	5.1	82
18	"Inverted" sodium-lithium electronegativity: polarity and metalation energies of organic and inorganic alkali-metal compounds. *Organometallics*, **1993**, 12, 853-859	3.8	34
17	The peculiar coordination of barium: ab initio study of the molecular and electronic structures of the Group II dihydride dimers M2H4 (M = magnesium, calcium, strontium, barium). *Journal of the American Chemical Society*, **1993**, 115, 11202-11208	16.4	30
16	Ab initio study of structures and stabilities of substituted lead compounds. Why is inorganic lead chemistry dominated by PbII but organolead chemistry by PbIV?. *Journal of the American Chemical Society*, **1993**, 115, 1061-1073	16.4	111
15	Gaseous Mercury(IV) Fluoride, HgF4: An Ab Initio Study. *Angewandte Chemie International Edition in English*, **1993**, 32, 861-863		59
14	Molekulares Quecksilber(IV)-fluorid, HgF4: eine ab-initio-Untersuchung. *Angewandte Chemie*, **1993**, 105, 952-954	3.6	18
13	Model calcium hydride CaH2(L) and calcium fluoride CaF2(L) complexes (L = neon, argon, krypton, xenon, carbon monoxide, nitrogen mol.): consequences of interactions between "inert-gas" ligands and floppy molecules. *The Journal of Physical Chemistry*, **1992**, 96, 9801-9805		18
12	The equilibrium structures of monomeric Group 2 and lanthanide(II) metallocenes MCp2 (M = calcium, strontium, barium, samarium, europium, ytterbium) studied by ab initio calculations. *Journal of the American Chemical Society*, **1992**, 114, 8202-8208	16.4	91
11	Do low-coordinated Group 1-3 cations Mn+Lm (Mn+ = potassium, rubidium cesium, calcium, strontium, barium, scandium, yttrium, lanthanum; L = ammonia, water, hydrogen fluoride; m = 1-3) with a formal noble-gas electron configuration favor regular or abnormal shapes?. *The Journal of*		56
10	Experimental and theoretical studies of alkaline-earth metal coordination: x-ray crystal structures of calcium, strontium, and barium carbazoles and ab initio model calculations. *Journal of the American Chemical Society*, **1992**, 114, 10880-10889	16.4	37
9	The ions MCp2+ (M = scandium, lanthanum): significantly bent sandwich species. *Organometallics*, **1992**, 11, 2765-2767	3.8	26

8	Relationships in the rotational barriers of all Group 14 ethane congeners H3X-YH3 (X, Y = C, Si, Ge, Sn, Pb). Comparisons of ab initio pseudopotential and all-electron results. *Journal of the American Chemical Society*, **1992**, 114, 6791-6797	16.4	80
7	The structural variations of monomeric alkaline earth MX2 compounds (M = calcium, strontium, barium; X = Li, BeH, BH2, CH3, NH2, OH, F). An ab initio pseudopotential study. *Journal of the American Chemical Society*, **1992**, 114, 491-497	16.4	97
6	The Structure and Stability Trends of Fluoro(methyl)plumbanes. *Angewandte Chemie International Edition in English*, **1992**, 31, 1224-1226		5
5	Struktur- und Stabilitätstendenzen bei Fluor(methyl)plumbanen. *Angewandte Chemie*, **1992**, 104, 1240-1242	3.6	2
4	The question of bending of the alkaline earth dihalides MX2 (M = beryllium, magnesium, calcium, strontium, barium; X = fluorine, chlorine, bromine, iodine). An ab initio pseudopotential study. *Journal of the American Chemical Society*, **1991**, 113, 6012-6020	16.4	159
3	Pseudopotential approaches to Ca, Sr, and Ba hydrides. Why are some alkaline earth MX2 compounds bent?. *Journal of Chemical Physics*, **1991**, 94, 1360-1366	3.9	502
2	Theoretical and experimental study of diamagnetic and paramagnetic products from thermal and light-induced alkyl transfer between zinc or magnesium dialkyls and 1,4-diaza-1,3-butadiene substrates. *Journal of the American Chemical Society*, **1991**, 113, 5606-5618	16.4	106
1	Pseudopotential calculations for methyl compounds of zinc and magnesium. *Journal of Computational Chemistry*, **1990**, 11, 1029-1037	3.5	20