Lothar Helm

List of Publications by Year
in descending order

79 papers	6,177 citations	71102 41 h-index	69250 77 g-index
84 all docs	84 docs citations	84 times ranked	5261 citing authors

#	Article	IF	Citations
1	Inorganic and Bioinorganic Solvent Exchange Mechanisms. Chemical Reviews, 2005, 105, 1923-1960.	47.7	667
2	Structural and Dynamic Parameters Obtained from17O NMR, EPR, and NMRD Studies of Monomeric and Dimeric Gd3+Complexes of Interest in Magnetic Resonance Imaging:Â An Integrated and Theoretically Self-Consistent Approach1. Journal of the American Chemical Society, 1996, 118, 9333-9346.	13.7	630
3	First Solvation Shell of the Cu(II) Aqua Ion: Evidence for Fivefold Coordination. Science, 2001, 291, 856-859.	12.6	358
4	Water-Soluble Gadofullerenes:Â Toward High-Relaxivity, pH-Responsive MRI Contrast Agents. Journal of the American Chemical Society, 2005, 127, 799-805.	13.7	341
5	Superparamagnetic gadonanotubes are high-performance MRI contrast agents. Chemical Communications, 2005, , 3915.	4.1	310
6	Relaxivity of MRI Contrast Agents. Topics in Current Chemistry, 2002, , 61-101.	4.0	168
7	Relaxivity in paramagnetic systems: Theory and mechanisms. Progress in Nuclear Magnetic Resonance Spectroscopy, 2006, 49, 45-64.	7.5	156
8	Water exchange on [Gd(H2O)8]3+ and [Gd(PDTA)(H2O)2]- in aqueous solution: A variable-pressure, -temperature and -magnetic field17O NMR study. Magnetic Resonance in Chemistry, 1993, 31, 1011-1020.	1.9	138
9	Gold Nanoparticles Functionalized with Gadolinium Chelates as High-Relaxivity MRI Contrast Agents. Journal of the American Chemical Society, 2009, 131, 10828-10829.	13.7	134
10	EPR Spectroscopy of MRI-Related Gd(III) Complexes:Â Simultaneous Analysis of Multiple Frequency and Temperature Spectra, Including Static and Transient Crystal Field Effects. Journal of the American Chemical Society, 2001, 123, 2637-2644.	13.7	129
11	High-pressure NMR kinetics. Part 34. Variable-temperature and variable-pressure NMR kinetic study of solvent exchange on hexaaquaruthenium(3+) and -(2+) and hexakis(acetonitrile)ruthenium(2+). Inorganic Chemistry, 1988, 27, 873-879.	4.0	125
12	Destroying Gadofullerene Aggregates by Salt Addition in Aqueous Solution of Gd@C60(OH)xand Gd@C60[C(COOH2)]10. Journal of the American Chemical Society, 2005, 127, 9368-9369.	13.7	119
13	Water Exchange on Hexaaquavanadium(III): a Variable-Temperature and Variable-Pressure17O-NMR Study at 1.4 and 4.7 Tesla. Helvetica Chimica Acta, 1985, 68, 508-521.	1.6	110
14	Rigid MIIL2Gd2III (M = Fe, Ru) Complexes of a Terpyridine-Based Heteroditopic Chelate:â€‰ A Class of Candidates for MRI Contrast Agents. Journal of the American Chemical Society, 2005, 127, 5147-5157.	13.7	98
15	Gd(DTPA-bisamide)alkyl Copolymers: A Hint for the Formation of MRI Contrast Agents with Very High Relaxivity. Chemistry - A European Journal, 1999, 5, 1202-1211.	3.3	97
16	Comparison of different methods for calculating the paramagnetic relaxation enhancement of nuclear spins as a function of the magnetic field. Journal of Chemical Physics, 2008, 128, 052315.	3.0	95
17	Optimization of gadolinium-based MRI contrast agents for high magnetic-field applications. Future Medicinal Chemistry, 2010, 2, 385-396.	2.3	95
18	A Highly Stable Gadolinium Complex with a Fast, Associative Mechanism of Water Exchange. Journal of the American Chemical Society, 2003, 125, 14274-14275.	13.7	81

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19	Hyperfine Coupling Constants on Innerâ€Sphere Water Molecules of Gd^{III}â€Based MRI Contrast Agents. ChemPhysChem, 2012, 13, 3640-3650.	2.1	80
20	Molecular Dynamics Simulations of MRI-Relevant GdIII Chelates: Direct Access to Outer-Sphere Relaxivity. Chemistry - A European Journal, 2001, 7, 600-610.	3.3	78
21	Physicochemical and MRI characterization of Gd3+-loaded polyamidoamine and hyperbranched dendrimers. Journal of Biological Inorganic Chemistry, 2007, 12, 406-420.	2.6	78
22	¹H and ¹⁷O NMR Relaxometric and Computational Study on Macrocyclic Mn(II) Complexes. Inorganic Chemistry, 2013, 52, 3268-3279.	4.0	77
23	WATER AND PROTON EXCHANGE PROCESSES ON METAL IONS. Advances in Inorganic Chemistry, 2005, 57, 327-379.	1.0	74
24	Coordination equilibriumâ€" a clue for fast water exchange on potential magnetic resonance imaging contrast agents?. , 1999, 37, 701-708.		73
25	A benzene-core trinuclear Gd^{III}complex: towards the optimization of relaxivity for MRI contrast agent applications at high magnetic field. Dalton Transactions, 2008, , 1195-1202.	3.3	72
26	Direct measurement of a prominent outer-sphere electron self-exchange: kinetic parameters for the hexaaquaruthenium(II)/(III) couple determined by oxygen-17 and ruthenium-99 NMR. Journal of the American Chemical Society, 1985, 107, 312-317.	13.7	68
27	Structure and Dynamics of a Trinuclear Gadolinium(III) Complex: The Effect of Intramolecular Electron Spin Relaxation on Its Proton Relaxivity1. Inorganic Chemistry, 1998, 37, 4104-4113.	4.0	63
28	Understanding Paramagnetic Relaxation Phenomena for Water-Soluble Gadofullerenes. Journal of Physical Chemistry C, 2007, 111, 5633-5639.	3.1	63
29	High pressure NMR kinetics. Part 30. Water exchange on hexaaquagallium(III): high-pressure evidence for a dissociative exchange mechanism. Journal of the American Chemical Society, 1987, 109, 4444-4450.	13.7	60
30	A High-Frequency EPR Study of Frozen Solutions of GdIIIComplexes:Â Straightforward Determination of the Zero-Field Splitting Parameters and Simulation of the NMRD Profiles. Journal of the American Chemical Society, 2006, 128, 7807-7816.	13.7	59
31	The effect of pyridinecarboxylate chelating groups on the stability and electronic relaxation of gadolinium complexes. Dalton Transactions, 2005, , 1129-1135.	3.3	58
32	Dinuclear, Bishydrated GdIIIPolyaminocarboxylates with a Rigid Xylene Core Display Remarkable Proton Relaxivities. Inorganic Chemistry, 2005, 44, 4747-4755.	4.0	58
33	SOLVENT EXCHANGE ON METAL IONS. Advances in Inorganic Chemistry, 2003, 54, 1-69.	1.0	56
34	Direct assessment of water exchange on a Gd(III) chelate bound to a protein. Journal of Biological Inorganic Chemistry, 1998, 3, 606-613.	2.6	51
35	Molecular Dynamics Simulation of [Gd(egta)(H2O)]â^' in Aqueous Solution: Internal Motions of the Poly(amino carboxylate) and Water Ligands, and Rotational Correlation Times. Chemistry - A European Journal, 2002, 8, 1031.	3.3	49
36	Quantum Chemical Investigation of Hyperfine Coupling Constants on First Coordination Sphere Water Molecule of Gadolinium(III) Aqua Complexes. Journal of Physical Chemistry A, 2005, 109, 10997-11005.	2.5	49

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37	Gadolinium (III) ion in liquid water: Structure, dynamics, and magnetic interactions from first principles. Journal of Chemical Physics, 2007, 127, 084506.	3.0	49
38	Relevance of the Ligand Exchange Rate and Mechanism of fac-[(CO)3M(H2O)3]+ (M = Mn, Tc, Re) Complexes for New Radiopharmaceuticals. Inorganic Chemistry, 2006, 45, 10378-10390.	4.0	48
39	Kinetics of Yttriumâ^'Ligand Complexation Monitored Using Hyperpolarized ⁸⁹Y as a Model for Gadolinium in Contrast Agents. Journal of the American Chemical Society, 2010, 132, 5006-5007.	13.7	48
40	A ruthenium-based metallostar: synthesis, sensitized luminescence and 1H relaxivity. Dalton Transactions, 2009, , 2088.	3.3	46
41	High pressure NMR kinetics. 29. Variable-temperature, -pressure, and -frequency oxygen-17 NMR study of water exchange on hexaaquatitanium(III): a limiting associative mechanism?. Inorganic Chemistry, 1987, 26, 1763-1768.	4.0	43
42	Multiexponential Electronic Spin Relaxation and Redfield's Limit in Gd(III) Complexes in Solution:Â Consequences for17O/1H NMR and EPR Simultaneous Analysis. Journal of the American Chemical Society, 2002, 124, 2042-2048.	13.7	42
43	Gadolinium(III) complexes of 1,4,7-triazacyclononane based picolinate ligands: simultaneous optimization of water exchange kinetics and electronic relaxation. Dalton Transactions, 2009, , 8033.	3.3	42
44	Gd(III) based MRI contrast agents: improved physical meaning in a combined analysis of EPR and NMR data?. Inorganic Chemistry Communication, 2002, 5, 811-815.	3.9	40
45	MD Simulations of Acyclic and Macrocyclic Gd3+-Based MRI Contrast Agents: Influence of the Internal Mobility on Water Proton Relaxivity. Chemistry - A European Journal, 2003, 9, 5468-5480.	3.3	40
46	Core spin-polarization correction in pseudopotential-based electronic structure calculations. Physical Review B, 2005, 71, .	3.2	39
47	Towards the Rational Design of MRI Contrast Agents: Electron Spin Relaxation Is Largely Unaffected by the Coordination Geometry of Gadolinium(III)â€"DOTAâ€Type Complexes. Chemistry - A European Journal, 2008, 14, 2658-2667.	3.3	39
48	EPR on aqueous Gd3+ complexes and a new analysis method considering both line widths and shifts. Physical Chemistry Chemical Physics, 2000, 2, 1311-1317.	2.8	36
49	Design of Gd(III)-Based Magnetic Resonance Imaging Contrast Agents:Â Static and Transient Zero-Field Splitting Contributions to the Electronic Relaxation and Their Impact on Relaxivity. Journal of Physical Chemistry B, 2007, 111, 832-840.	2.6	34
50	Unexpected Aggregation of Neutral, Xylene-Cored Dinuclear GdIII Chelates in Aqueous Solution. Chemistry - A European Journal, 2006, 12, 6841-6851.	3.3	33
51	In vivo MRI assessment of a novel Gd^{III}â€based contrast agent designed for high magnetic field applications. Contrast Media and Molecular Imaging, 2008, 3, 78-85.	0.8	33
52	Ligand exchange and complex formation kinetics studied by NMR exemplified on fac-[(CO)3M(H2O)]+ (M=Mn, Tc, Re). Coordination Chemistry Reviews, 2008, 252, 2346-2361.	18.8	33
53	17O-NMR, EPR and NMRD Characterization of [Gd(DTPA-BMEA)(H2O)]: A Neutral MRI Contrast Agent. European Journal of Inorganic Chemistry, 1998, 1998, 2017-2021.	2.0	32
54	Physicochemical Properties of the High-Field MRI-Relevant [Gd(DTTA-Me)(H₂O)₂]^{â^'} Complex. Inorganic Chemistry, 2008, 47, 8357-8366.	4.0	32

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55	Gadolinium complexes of monophosphinic acid DOTA derivatives conjugated to cyclodextrin scaffolds: efficient MRI contrast agents for higher magnetic fields. Dalton Transactions, 2012, 41, 13509.	3.3	32
56	New Bisaqua Picolinate-Based Gadolinium Complexes as MRI Contrast Agents with Substantial High-Field Relaxivities. European Journal of Inorganic Chemistry, 2012, 2012, 2049-2061.	2.0	30
57	Nuclear Spin Relaxation Parameters of MRI Contrast Agents â€“ Insight from Quantum Mechanical Calculations. European Journal of Inorganic Chemistry, 2008, 2008, 201-211.	2.0	28
58	8S paramagnetic centres in molecular assemblies: possible effect of their proximity on the water proton relaxivity. Magnetic Resonance in Chemistry, 2003, 41, 794-799.	1.9	27
59	O17 nuclear quadrupole coupling constants of water bound to a metal ion: A gadolinium(III) case study. Journal of Chemical Physics, 2006, 125, 054503.	3.0	23
60	Synthesis, complexation and NMR relaxation properties of Gd3+ complexes of Mes(DO3A)3. Dalton Transactions, 2011, 40, 4260.	3.3	23
61	Gd(DOTAlaP): Exploring the Boundaries of Fast Water Exchange in Gadolinium-Based Magnetic Resonance Imaging Contrast Agents. Inorganic Chemistry, 2014, 53, 6985-6994.	4.0	23
62	Multiple-Frequency EPR Spectra of Two Aqueous Gd3+Polyamino Polypyridine Carboxylate Complexes:Â A Study of High Field Effects. Journal of Physical Chemistry A, 2007, 111, 5399-5407.	2.5	20
63	Gold nanoparticles functionalised with fast water exchanging Gd³⁺ chelates: linker effects on the relaxivity. Dalton Transactions, 2015, 44, 4016-4031.	3.3	19
64	Selfâ€Assembled Nanomicelles as MRI Bloodâ€Pool Contrast Agent. Chemistry - A European Journal, 2018, 24, 1348-1357.	3.3	19
65	MRI micelles self-assembled from synthetic gadolinium-based nano building blocks. Chemical Communications, 2019, 55, 945-948.	4.1	19
66	Multipleâ€Frequency and Variableâ€Temperature EPR Study of Gadolinium(III) Complexes with Polyaminocarboxylates: Analysis and Comparison of the Magnetically Dilute Powder and the Frozenâ€Solution Spectra. Helvetica Chimica Acta, 2009, 92, 2173-2185.	1.6	17
67	Hyperfine interactions in aqueous solution of Cr3+: an ab initio molecular dynamics study. Theoretical Chemistry Accounts, 2006, 115, 190-195.	1.4	14
68	Gd(III)â€EPTPAC₁₆, a new selfâ€assembling potential liver MRI contrast agent: in vitro characterization and in vivo animal imaging studies. NMR in Biomedicine, 2008, 21, 322-336.	2.8	14
69	Dinuclear DOTAâ€Based Gd^{III} Chelates â€“ Revisiting a Straightforward Strategy for Relaxivity Improvement. European Journal of Inorganic Chemistry, 2015, 2015, 1579-1591.	2.0	12
70	Complexation of [Gd(DTTAâ€“Me)(H₂O)₂]^{â^'} by Fluoride and Its Consequences to Water Exchange. Inorganic Chemistry, 2016, 55, 6231-6239.	4.0	9
71	The Periodic Table and Kinetics?. Chimia, 2019, 73, 179-184.	0.6	9
72	H₅EPTPACH₂OH: Synthesis, Relaxometric Characterization and ¹H NMR Spectroscopic Studies on the Solution Dynamics of Its Ln^{III} Complexes. European Journal of Inorganic Chemistry, 2007, 2007, 5489-5499.	2.0	8

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73	Dynamic aggregation of the mid-sized gadolinium complex {Ph4[Gd(DTTA)(H2O)2]â˜ 3}. Journal of Biological Inorganic Chemistry, 2014, 19, 145-159.	2.6	8
74	Water-Exchange Study Revealed Unexpected Substitution Behavior of [(CO)2(NO)Re(H2O)3]2+in Aqueous Media. Inorganic Chemistry, 2006, 45, 4199-4204.	4.0	7
75	PEGylated DOTAâ€AHAâ€Based Gd^{III} Chelates: A Relaxometric Study. European Journal of Inorganic Chemistry, 2015, 2015, 4798-4809.	2.0	5
76	Carbazole as Linker for Dinuclear Gadoliniumâ€Based MRI Contrast Agents. European Journal of Inorganic Chemistry, 2017, 2017, 5403-5412.	2.0	5
77	Molecular Dynamics of Gd(III) Complexes in Aqueous Solution by HF EPR. Biological Magnetic Resonance, 2004, , 207-247.	0.4	5
78	The Challenge of T1 Contrast Agents for High-Magnetic Field MRI. Chimia, 2011, 65, 696.	0.6	3
79	PEGylated DOTA-AHA-Based GdIIIChelates: A Relaxometric Study. European Journal of Inorganic Chemistry, 2015, 2015, 4784-4784.	2.0	0