

Alain Borel

List of Publications by Year in descending order

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1,978
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304368

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docs citations

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2325
citing authors

#	ARTICLE	IF	CITATIONS
1	Water-Soluble Gadofullerenes: Toward High-Relaxivity, pH-Responsive MRI Contrast Agents. <i>Journal of the American Chemical Society</i> , 2005, 127, 799-805.	6.6	341
2	ChemCalc: A Building Block for Tomorrow's Chemical Infrastructure. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1223-1228.	2.5	316
3	High Relaxivity Confined to a Small Molecular Space: A Metallostar-Based, Potential MRI Contrast Agent. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 1480-1484.	7.2	149
4	EPR Spectroscopy of MRI-Related Gd(III) Complexes: Simultaneous Analysis of Multiple Frequency and Temperature Spectra, Including Static and Transient Crystal Field Effects. <i>Journal of the American Chemical Society</i> , 2001, 123, 2637-2644.	6.6	129
5	A Starburst-Shaped Heterometallic Compound Incorporating Six Densely Packed Gd ³⁺ Ions. <i>Chemistry - A European Journal</i> , 2006, 12, 989-1003.	1.7	112
6	Molecular Dynamics Simulations of MRI-Relevant Gd(III) Chelates: Direct Access to Outer-Sphere Relaxivity. <i>Chemistry - A European Journal</i> , 2001, 7, 600-610.	1.7	78
7	A Multinuclear NMR Study on the Structure and Dynamics of Lanthanide(III) Complexes of the Poly(amino carboxylate) EGTA ⁴⁻ in Aqueous Solution. <i>Inorganic Chemistry</i> , 1997, 36, 5104-5112.	1.9	74
8	A general approach to the electronic spin relaxation of Gd(III) complexes in solutions. Monte Carlo simulations beyond the Redfield limit. <i>Journal of Chemical Physics</i> , 2001, 115, 7554-7563.	1.2	73
9	How Does Internal Motion Influence the Relaxation of the Water Protons in Ln(III)DOTA-like Complexes?. <i>Journal of the American Chemical Society</i> , 2002, 124, 710-716.	6.6	70
10	A High-Frequency EPR Study of Frozen Solutions of Gd(III) Complexes: Straightforward Determination of the Zero-Field Splitting Parameters and Simulation of the NMRD Profiles. <i>Journal of the American Chemical Society</i> , 2006, 128, 7807-7816.	6.6	59
11	The effect of pyridinecarboxylate chelating groups on the stability and electronic relaxation of gadolinium complexes. <i>Dalton Transactions</i> , 2005, , 1129-1135.	1.6	58
12	A ruthenium-based metallostar: synthesis, sensitized luminescence and ¹ H relaxivity. <i>Dalton Transactions</i> , 2009, , 2088.	1.6	46
13	Multixponential Electronic Spin Relaxation and Redfield's Limit in Gd(III) Complexes in Solution: Consequences for ¹⁷ O/ ¹ H NMR and EPR Simultaneous Analysis. <i>Journal of the American Chemical Society</i> , 2002, 124, 2042-2048.	6.6	42
14	Hybrid ligand-field theory/quantum chemical calculation of the fine structure and ZFS in lanthanide(III) complexes. <i>Chemical Physics Letters</i> , 2004, 383, 584-591.	1.2	42
15	Gd(III) based MRI contrast agents: improved physical meaning in a combined analysis of EPR and NMR data?. <i>Inorganic Chemistry Communication</i> , 2002, 5, 811-815.	1.8	40
16	MD Simulations of Acyclic and Macrocyclic Gd ³⁺ -Based MRI Contrast Agents: Influence of the Internal Mobility on Water Proton Relaxivity. <i>Chemistry - A European Journal</i> , 2003, 9, 5468-5480.	1.7	40
17	Towards the Rational Design of MRI Contrast Agents: Electron Spin Relaxation Is Largely Unaffected by the Coordination Geometry of Gadolinium(III)DOTA-type Complexes. <i>Chemistry - A European Journal</i> , 2008, 14, 2658-2667.	1.7	39
18	Variable Temperature and EPR Frequency Study of Two Aqueous Gd(III) Complexes with Unprecedented Sharp Lines. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12434-12438.	1.1	37

#	ARTICLE	IF	CITATIONS
19	EPR on aqueous Gd ³⁺ complexes and a new analysis method considering both line widths and shifts. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 1311-1317.	1.3	36
20	T1e in Four Gd ³⁺ Chelates: LODEPR Measurements and Models for Electron Spin Relaxation. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6229-6231.	1.1	34
21	Design of Gd(III)-Based Magnetic Resonance Imaging Contrast Agents: Static and Transient Zero-Field Splitting Contributions to the Electronic Relaxation and Their Impact on Relaxivity. <i>Journal of Physical Chemistry B</i> , 2007, 111, 832-840.	1.2	34
22	A Theoretical Characterization of Covalency in Rare Earth Complexes through Their Absorption Electronic Properties: f-f Transitions. <i>Inorganic Chemistry</i> , 2006, 45, 7382-7388.	1.9	33
23	High Relaxivity Confined to a Small Molecular Space: A Metallostar-Based, Potential MRI Contrast Agent. <i>Angewandte Chemie</i> , 2005, 117, 1504-1508.	1.6	20
24	Multiple-Frequency EPR Spectra of Two Aqueous Gd ³⁺ -Polyamino Polypyridine Carboxylate Complexes: A Study of High Field Effects. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5399-5407.	1.1	20
25	Multiple-Frequency and Variable-Temperature EPR Study of Gadolinium(III) Complexes with Polyaminocarboxylates: Analysis and Comparison of the Magnetically Dilute Powder and the Frozen-Solution Spectra. <i>Helvetica Chimica Acta</i> , 2009, 92, 2173-2185.	1.0	17
26	Electronic fine structure calculation of [Gd(DOTA)(H ₂ O)] ³⁺ using LF-DFT: The zero field splitting. <i>Comptes Rendus Chimie</i> , 2012, 15, 250-254.	0.2	13
27	Stochastic Liouville equation treatment of the electron paramagnetic resonance line shape of an S-state ion in solution. <i>Journal of Chemical Physics</i> , 2007, 126, 054510.	1.2	10
28	Multiplets of free d- and f-metal ions: A systematic DFT study. <i>Computational and Theoretical Chemistry</i> , 2006, 762, 93-107.	1.5	8
29	Molecular Dynamics of Gd(III) Complexes in Aqueous Solution by HF EPR. <i>Biological Magnetic Resonance</i> , 2004, , 207-247.	0.4	5
30	Site Selective Functionalization of Fluorinated Nitrogen Heterocycles. <i>ACS Symposium Series</i> , 2009, , 23-35.	0.5	3
31	Molecular Dynamics Simulations of the Internal Mobility of Gd ³⁺ -Based MRI Contrast Agents: Consequences for Water Proton Relaxivity. <i>Chimia</i> , 2004, 58, 200-203.	0.3	0
32	Molecular Dynamics of Gd(III) Complexes in Aqueous Solution by HF EPR. <i>ChemInform</i> , 2005, 36, no.	0.1	0