Alain Borel

List of Publications by Year
in descending order

32	1,978	304368	454577
papers	citations	22 h-index	30 g-index

33	33	33	2325
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	ChemCalc: A Building Block for Tomorrowâ€™s Chemical Infrastructure. Journal of Chemical Information and Modeling, 2013, 53, 1223-1228.	2.5	316
2	Electronic fine structure calculation of [Gd(DOTA)(H2O)]â€“ using LF-DFT: The zero field splitting. Comptes Rendus Chimie, 2012, 15, 250-254.	0.2	13
3	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.	1.0	17
4	A ruthenium-based metallostar: synthesis, sensitized luminescence and 1H relaxivity. Dalton Transactions, 2009, , 2088.	1.6	46
5	Site Selective Functionalization of Fluorinated Nitrogen Heterocycles. ACS Symposium Series, 2009, , 23-35.	0.5	3
6	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.	1.7	39
7	Stochastic Liouville equation treatment of the electron paramagnetic resonance line shape of an S-state ion in solution. Journal of Chemical Physics, 2007, 126, 054510.	1.2	10
8	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.	1.2	34
9	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.	1.1	20
10	A Theoretical Characterization of Covalency in Rare Earth Complexes through Their Absorption Electronic Properties:â€‰ fâ^’f Transitions. Inorganic Chemistry, 2006, 45, 7382-7388.	1.9	33
11	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.	6.6	59
12	Variable Temperature and EPR Frequency Study of Two Aqueous Gd(III) Complexes with Unprecedented Sharp Lines. Journal of Physical Chemistry A, 2006, 110, 12434-12438.	1.1	37
13	Multiplets of free d- and f-metal ions: A systematic DFT study. Computational and Theoretical Chemistry, 2006, 762, 93-107.	1.5	8
14	A Starburst-Shaped Heterometallic Compound Incorporating Six Densely Packed Gd3+ Ions. Chemistry - A European Journal, 2006, 12, 989-1003.	1.7	112
15	The effect of pyridinecarboxylate chelating groups on the stability and electronic relaxation of gadolinium complexes. Dalton Transactions, 2005, , 1129-1135.	1.6	58
16	High Relaxivity Confined to a Small Molecular Space: A Metallostar-Based, Potential MRI Contrast Agent. Angewandte Chemie - International Edition, 2005, 44, 1480-1484.	7.2	149
17	High Relaxivity Confined to a Small Molecular Space: A Metallostar-Based, Potential MRI Contrast Agent. Angewandte Chemie, 2005, 117, 1504-1508.	1.6	20
18	Molecular Dynamics of Gd(III) Complexes in Aqueous Solution by HF EPR. ChemInform, 2005, 36, no.	0.1	0

#	Article	IF	Citations
19	Water-Soluble Gadofullerenes:Â Toward High-Relaxivity, pH-Responsive MRI Contrast Agents. Journal of the American Chemical Society, 2005, 127, 799-805.	6.6	341
20	Hybrid ligand-field theory/quantum chemical calculation of the fine structure and ZFS in lanthanide(III) complexes. Chemical Physics Letters, 2004, 383, 584-591.	1.2	42
21	Molecular Dynamics Simulations of the Internal Mobility of Gd³⁺-Based MRI Contrast Agents: Consequences for Water Proton Relaxivity. Chimia, 2004, 58, 200-203.	0.3	0
22	Molecular Dynamics of Gd(III) Complexes in Aqueous Solution by HF EPR. Biological Magnetic Resonance, 2004, , 207-247.	0.4	5
23	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.	1.7	40
24	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.	6.6	42
25	How Does Internal Motion Influence the Relaxation of the Water Protons in LnIIIDOTA-like Complexes?. Journal of the American Chemical Society, 2002, 124, 710-716.	6.6	70
26	T1e in Four Gd3+ Chelates:â€‰LODEPR Measurements and Models for Electron Spin Relaxation. Journal of Physical Chemistry A, 2002, 106, 6229-6231.	1.1	34
27	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.	1.8	40
28	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.	6.6	129
29	Molecular Dynamics Simulations of MRI-Relevant GdIII Chelates: Direct Access to Outer-Sphere Relaxivity. Chemistry - A European Journal, 2001, 7, 600-610.	1.7	78
30	A general approach to the electronic spin relaxation of Gd(III) complexes in solutions. Monte Carlo simulations beyond the Redfield limit. Journal of Chemical Physics, 2001, 115, 7554-7563.	1.2	73
31	EPR on aqueous Gd3+ complexes and a new analysis method considering both line widths and shifts. Physical Chemistry Chemical Physics, 2000, 2, 1311-1317.	1.3	36
32	A Multinuclear NMR Study on the Structure and Dynamics of Lanthanide(III) Complexes of the Poly(amino carboxylate) EGTA4-in Aqueous Solution. Inorganic Chemistry, 1997, 36, 5104-5112.	1.9	74