

Liviu Ungur

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	<sc>Molcas</sc> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. <i>Journal of Computational Chemistry</i> , 2016, 37, 506-541.	1.5	1,317
2	A Stable Pentagonal Bipyramidal Dy(III) Single-Ion Magnet with a Record Magnetization Reversal Barrier over 1000 K. <i>Journal of the American Chemical Society</i> , 2016, 138, 5441-5450.	6.6	904
3	Symmetry-Supported Magnetic Blocking at 20 K in Pentagonal Bipyramidal Dy(III) Single-Ion Magnets. <i>Journal of the American Chemical Society</i> , 2016, 138, 2829-2837.	6.6	728
4	Strong Axiality and Ising Exchange Interaction Suppress Zero-Field Tunneling of Magnetization of an Asymmetric Dy ₂ Single-Molecule Magnet. <i>Journal of the American Chemical Society</i> , 2011, 133, 11948-11951.	6.6	670
5	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5925-5964.	2.3	661
6	Magnetic relaxation pathways in lanthanide single-molecule magnets. <i>Nature Chemistry</i> , 2013, 5, 673-678.	6.6	649
7	The Origin of Nonmagnetic Kramers Doublets in the Ground State of Dysprosium Triangles: Evidence for a Toroidal Magnetic Moment. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 4126-4129.	7.2	610
8	<i>Ab initio</i> calculation of anisotropic magnetic properties of complexes. I. Unique definition of pseudospin Hamiltonians and their derivation. <i>Journal of Chemical Physics</i> , 2012, 137, 064112.	1.2	573
9	A Polynuclear Lanthanide Single-Molecule Magnet with a Record Anisotropic Barrier. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 9489-9492.	7.2	557
10	Single-Molecule Magnet Behavior for an Antiferromagnetically Superexchange-Coupled Dinuclear Dysprosium(III) Complex. <i>Journal of the American Chemical Society</i> , 2011, 133, 5319-5328.	6.6	541
11	Switching the anisotropy barrier of a single-ion magnet by symmetry change from quasi-D5h to quasi-Oh. <i>Chemical Science</i> , 2013, 4, 3310.	3.7	469
12	Structure, Magnetism, and Theoretical Study of a Mixed-Valence Co ^{II} ₃ Co ^{III} ₄ Heptanuclear Wheel: Lack of SMM Behavior despite Negative Magnetic Anisotropy. <i>Journal of the American Chemical Society</i> , 2008, 130, 12445-12455.	6.6	442
13	Fine-tuning the Local Symmetry to Attain Record Blocking Temperature and Magnetic Remanence in a Single-Ion Magnet. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 4413-4417.	7.2	370
14	Strategies toward High-Temperature Lanthanide-Based Single-Molecule Magnets. <i>Inorganic Chemistry</i> , 2016, 55, 10043-10056.	1.9	342
15	Magnetic anisotropy in the excited states of low symmetry lanthanide complexes. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20086.	1.3	333
16	<i>Ab initio</i> investigation of the non-collinear magnetic structure and the lowest magnetic excitations in dysprosium triangles. <i>New Journal of Chemistry</i> , 2009, 33, 1224.	1.4	332
17	The active site of low-temperature methane hydroxylation in iron-containing zeolites. <i>Nature</i> , 2016, 536, 317-321.	13.7	331
18	Single-molecule toroids in Ising-type lanthanide molecular clusters. <i>Chemical Society Reviews</i> , 2014, 43, 6894-6905.	18.7	325

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19	Modern quantum chemistry with [Open]Molcas. <i>Journal of Chemical Physics</i> , 2020, 152, 214117.	1.2	281
20	Coupling Strategies to Enhance Single-Molecule Magnet Properties of Erbium ^{III} -Cyclooctatetraenyl Complexes. <i>Journal of the American Chemical Society</i> , 2014, 136, 8003-8010.	6.6	278
21	Coexistence of Distinct Single-Ion and Exchange-Based Mechanisms for Blocking of Magnetization in a Co ^{II} Dy ^{II} Single-Molecule Magnet. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 7550-7554.	7.2	277
22	An Octanuclear [Cr ^{III} Dy ^{III}] ₃ 3d-4f Single-Molecule Magnet. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 7583-7587.	7.2	256
23	A High Anisotropy Barrier in a Sulfur-Bridged Organodysprosium Single-Molecule Magnet. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 6976-6980.	7.2	254
24	Interplay of Strongly Anisotropic Metal Ions in Magnetic Blocking of Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 6328-6337.	1.9	239
25	Ab Initio Crystal Field for Lanthanides. <i>Chemistry - A European Journal</i> , 2017, 23, 3708-3718.	1.7	239
26	A Heterometallic Fe ^{II} -Dy ^{III} Single-Molecule Magnet with a Record Anisotropy Barrier. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 12966-12970.	7.2	235
27	A Non-sandwiched Macrocyclic Monolanthanide Single-Molecule Magnet: The Key Role of Axiality. <i>Chemistry - A European Journal</i> , 2011, 17, 4362-4365.	1.7	227
28	A Six-Coordinate Ytterbium Complex Exhibiting Easy-Plane Anisotropy and Field-Induced Single-Ion Magnet Behavior. <i>Inorganic Chemistry</i> , 2012, 51, 8538-8544.	1.9	221
29	Coupling Dy ³⁺ Triangles to Maximize the Toroidal Moment. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 12767-12771.	7.2	207
30	First Heterotrimetallic {3d-4d-4f} Single Chain Magnet, Constructed from Anisotropic High-Spin, Heterometallic Nodes and Paramagnetic Spacers. <i>Chemistry - A European Journal</i> , 2009, 15, 11808-11814.	1.7	205
31	The First {Dy ⁴⁺ } Single-Molecule Magnet with a Toroidal Magnetic Moment in the Ground State. <i>Inorganic Chemistry</i> , 2012, 51, 1233-1235.	1.9	191
32	An Organometallic Building Block Approach To Produce a Multidecker 4f Single-Molecule Magnet. <i>Journal of the American Chemical Society</i> , 2013, 135, 3502-3510.	6.6	189
33	Pursuit of Record Breaking Energy Barriers: A Study of Magnetic Axiality in Diamide Ligated Dy ^{III} Single-Molecule Magnets. <i>Journal of the American Chemical Society</i> , 2017, 139, 1420-1423.	6.6	186
34	A single-molecule magnet assembly exhibiting a dielectric transition at 470 K. <i>Chemical Science</i> , 2012, 3, 3366.	3.7	175
35	Modifying the properties of 4f single-ion magnets by peripheral ligand functionalisation. <i>Chemical Science</i> , 2014, 5, 1650-1660.	3.7	159
36	Net Toroidal Magnetic Moment in the Ground State of a {Dy ⁶⁺ }-Triethanolamine Ring. <i>Journal of the American Chemical Society</i> , 2012, 134, 18554-18557.	6.6	157

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37	Supramolecular architectures for controlling slow magnetic relaxation in field-induced single-molecule magnets. <i>Chemical Science</i> , 2012, 3, 2158.	3.7	155
38	Heterometallic Tetranuclear $[Ln^{III}_2Co^{II}_2]$ Complexes Including Suppression of Quantum Tunneling of Magnetization in the $[Dy^{III}_2Co^{II}_2]$ Single Molecule Magnet. <i>Inorganic Chemistry</i> , 2012, 51, 11873-11881.	1.9	154
39	Heterometallic CuII/DyIII 1D chiral polymers: chirogenesis and exchange coupling of toroidal moments in trinuclear Dy ³ single molecule magnets. <i>Chemical Science</i> , 2012, 3, 1169.	3.7	146
40	Electronic Structure and Slow Magnetic Relaxation of Low-Coordinate Cyclic Alkyl(amino) Carbene Stabilized Iron(I) Complexes. <i>Journal of the American Chemical Society</i> , 2014, 136, 11964-11971.	6.6	145
41	An NCN-pincer ligand dysprosium single-ion magnet showing magnetic relaxation via the second excited state. <i>Scientific Reports</i> , 2014, 4, 5471.	1.6	138
42	Influencing the properties of dysprosium single-molecule magnets with phosphorus donor ligands. <i>Nature Communications</i> , 2015, 6, 7492.	5.8	126
43	Structure, Magnetism and Theory of a Family of Nonanuclear $Cu^{II}_5Ln^{III}_4$ "Triethanolamine Clusters Displaying Single-Molecule Magnet Behaviour. <i>Chemistry - A European Journal</i> , 2011, 17, 9209-9218.	1.7	114
44	From a Dy(III) Single Molecule Magnet (SMM) to a Ferromagnetic $[Mn(II)Dy(III)Mn(II)]$ Trinuclear Complex. <i>Inorganic Chemistry</i> , 2012, 51, 9589-9597.	1.9	112
45	Spectroscopic determination of crystal field splittings in lanthanide double deckers. <i>Chemical Science</i> , 2014, 5, 3287.	3.7	111
46	Symmetry related $[Dy^{III}_6Mn^{III}_{12}]$ cores with different magnetic anisotropies. <i>Chemical Science</i> , 2011, 2, 1268.	3.7	108
47	Dynamic Magnetic and Optical Insight into a High Performance Pentagonal Bipyramidal Dy^{III} Single-Molecule Magnet. <i>Chemistry - A European Journal</i> , 2017, 23, 5708-5715.	1.7	96
48	Pure Trinuclear 4% of Single-Molecule Magnets: Synthesis, Structures, Magnetism and Ab Initio Investigation. <i>Chemistry - A European Journal</i> , 2011, 17, 2458-2466.	1.7	93
49	Heterometallic 3d-4f Single-Molecule Magnets: Ligand and Metal Ion Influences on the Magnetic Relaxation. <i>Inorganic Chemistry</i> , 2015, 54, 3631-3642.	1.9	92
50	Single-Molecule Magnetism in a Family of $\{Co^{III}_2Dy^{III}_2\}$ Butterfly Complexes: Effects of Ligand Replacement on the Dynamics of Magnetic Relaxation. <i>Inorganic Chemistry</i> , 2014, 53, 4303-4315.	1.9	88
51	Tuning the Magnetic Interactions and Relaxation Dynamics of Dy^{II}_2 Single-Molecule Magnets. <i>Chemistry - A European Journal</i> , 2015, 21, 14099-14106.	1.7	87
52	Desolvation-Driven 100-Fold Slow-down of Tunneling Relaxation Rate in Co(II)-Dy(III) Single-Molecule Magnets through a Single-Crystal-to-Single-Crystal Process. <i>Scientific Reports</i> , 2015, 5, 16621.	1.6	84
53	Synthesis and Characterization of a Two-Coordinate Manganese Complex and its Reaction with Molecular Hydrogen at Room Temperature. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 11817-11821.	7.2	78
54	A hydride-ligated dysprosium single-molecule magnet. <i>Chemical Communications</i> , 2013, 49, 901-903.	2.2	75

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55	Ytterbium can relax slowly too: a field-induced Yb ₂ single-molecule magnet. Dalton Transactions, 2012, 41, 12349.	1.6	73
56	Multitechnique investigation of Dy ₃ – implications for coupled lanthanide clusters. Chemical Science, 2016, 7, 4347-4354.	3.7	70
57	Exchange coupling and single molecule magnetism in redox-active tetraoxolene-bridged dilanthanide complexes. Chemical Science, 2018, 9, 1221-1230.	3.7	70
58	By Design: A Macrocyclic 3d ⁴ f Single-Molecule Magnet with Quantifiable Zero-Field Slow Relaxation of Magnetization. Inorganic Chemistry, 2013, 52, 3236-3240.	1.9	69
59	Key Role of Frustration in Suppression of Magnetization Blocking in Single-Molecule Magnets. Journal of Physical Chemistry Letters, 2013, 4, 3565-3569.	2.1	67
60	Angular-Resolved Magnetometry Beyond Triclinic Crystals: Out-of-Equilibrium Studies of Cp*ErCOT Single-Molecule Magnet. Chemistry - A European Journal, 2013, 19, 13726-13731.	1.7	67
61	Relaxations in heterolanthanide dinuclear single-molecule magnets. Chemical Communications, 2013, 49, 158-160.	2.2	66
62	A Rare $\frac{1}{4}$ -Centred Dy ₄ Tetrahedron with Coordination-Induced Local Chirality and Single-Molecule Magnet Behaviour. European Journal of Inorganic Chemistry, 2011, 2011, 1535-1539.	1.0	65
63	Observation of unusual slow-relaxation of the magnetisation in a Gd-EDTA chelate. Dalton Transactions, 2015, 44, 20321-20325.	1.6	62
64	A dinuclear cobalt(ii) complex of calix[8]arenes exhibiting strong magnetic anisotropy. Dalton Transactions, 2007, , 4582.	1.6	58
65	A Catalyst with Two-Coordinate Nickel: Theoretical and Catalytic Studies. European Journal of Inorganic Chemistry, 2014, 2014, 818-823.	1.0	57
66	Synthesis and Magnetic Properties of a New Family of Macrocyclic MII3LnIII Complexes: Insights into the Effect of Subtle Chemical Modification on Single-Molecule Magnet Behavior. Inorganic Chemistry, 2012, 51, 10603-10612.	1.9	56
67	Magnetic Relaxation in Single-Electron Single-Ion Cerium(III) Magnets: Insights from Ab Initio Calculations. Chemistry - A European Journal, 2015, 21, 13812-13819.	1.7	56
68	Cycloheptatrienyl trianion: an elusive bridge in the search of exchange coupled dinuclear organolanthanide single-molecule magnets. Chemical Science, 2017, 8, 231-240.	3.7	56
69	Stabilization of a Cobalt-Cobalt Bond by Two Cyclic Alkyl Amino Carbenes. Journal of the American Chemical Society, 2014, 136, 1770-1773.	6.6	55
70	Giant exchange interaction in mixed lanthanides. Scientific Reports, 2016, 6, 24046.	1.6	54
71	Tetraanionic Biphenyl Lanthanide Complexes as Single-Molecule Magnets. Inorganic Chemistry, 2015, 54, 2374-2382.	1.9	49
72	Determination of the electronic structure of a dinuclear dysprosium single molecule magnet without symmetry idealization. Chemical Science, 2019, 10, 2101-2110.	3.7	48

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73	Chemical tuning of the magnetic relaxation in dysprosium(III) mononuclear complexes. Dalton Transactions, 2014, 43, 12146-12149.	1.6	45
74	Field-Induced Multiple Relaxation Mechanism of Co ^{III} ₂ Dy ^{III} Compound with the Dysprosium Ion in a Low-Symmetrical Environment. Inorganic Chemistry, 2014, 53, 12658-12663.	1.9	42
75	Strong ferromagnetic exchange coupling in a {NiII ₄ } cluster mediated through an air-stable tetrazine-based radical anion. Chemical Communications, 2017, 53, 8660-8663.	2.2	40
76	Synthesis, Crystal Structures, Magnetic Properties, and Theoretical Investigation of a New Series of Ni ^{II} -Ln ^{III} -W ^V Heterotrimetallics: Understanding the SMM Behavior of Mixed Polynuclear Complexes. Inorganic Chemistry, 2016, 55, 12158-12171.	1.9	39
77	Gold-Catalyzed Post-Ugi Ipso-Cyclization with Switchable Diastereoselectivity. Journal of Organic Chemistry, 2018, 83, 8170-8182.	1.7	39
78	Hysteresis in the ground and excited spin state up to 10 T of a [Mn ^{III} 6Mn ^{III}] ₃₊ triple-salen single-molecule magnet. Chemical Science, 2012, 3, 2868.	3.7	37
79	A Spectroscopic Investigation of Magnetic Exchange Between Highly Anisotropic Spin Centers. Angewandte Chemie - International Edition, 2011, 50, 4007-4011.	7.2	33
80	Single-Molecule Toric Design through Magnetic Exchange Coupling. Matter, 2020, 2, 1481-1493.	5.0	32
81	An Inconspicuous Six-Coordinate Neutral Dy ^{III} Single-Ion Magnet with Remarkable Magnetic Anisotropy and Stability. Inorganic Chemistry, 2020, 59, 7158-7166.	1.9	31
82	Ein heterometallischer Fe ^{II} -Dy ^{III} -Einzelmolekülmagnet mit Rekord-Anisotropiebarriere. Angewandte Chemie, 2014, 126, 13180-13184.	1.6	30
83	Magnetic Anisotropy in Divalent Lanthanide Compounds. Angewandte Chemie - International Edition, 2020, 59, 12720-12724.	7.2	29
84	Ein achtkerniger [Cr ^{III} ₄ Dy ^{III} ₄]-Einzelmolekülmagnet. Angewandte Chemie, 2010, 122, 7746-7750.	1.6	25
85	Synthesis, structure, magnetism and theoretical study of a series of complexes with a decanuclear core [Ln ⁽ⁱⁱⁱ⁾ 2Cu ⁽ⁱⁱ⁾] ₈ (Ln = Y, Gd, Tb, Dy). New Journal of Chemistry, 2011, 35, 1270.	1.4	25
86	Exchange Interactions Switch Tunneling: A Comparative Experimental and Theoretical Study on Relaxation Dynamics by Targeted Metal Ion Replacement. Chemistry - A European Journal, 2018, 24, 9928-9939.	1.7	21
87	Negative g Factors, Berry Phases, and Magnetic Properties of Complexes. Physical Review Letters, 2012, 109, 246403.	2.9	20
88	Highly Oxidized States of Phthalocyaninato Terbium(III) Multiple-Decker Complexes Showing Structural Deformations, Biradical Properties and Decreases in Magnetic Anisotropy. Chemistry - A European Journal, 2020, 26, 8621-8630.	1.7	19
89	A Family of Lanthanide Hydroxo Carboxylates with 1D Polymeric Topology and Ln ₄ Butterfly Core Exhibits Switchable Supramolecular Arrangement. Inorganic Chemistry, 2021, 60, 8049-8061.	1.9	18
90	Coexistence of Spin-Lattice Relaxation and Phonon Bottleneck Processes in Gd ^{III} -Phthalocyaninato Triple-Decker Complexes under Highly Diluted Conditions. Chemistry - A European Journal, 2020, 26, 8076-8082.	1.7	16

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91	Magnetization Blocking in Fe ₂ ^{III}Dy ₂ ^{III} Molecular Magnets: Ab Initio Calculations and EPR Spectroscopy. Chemistry - A European Journal, 2018, 24, 16652-16661.	1.7	15
92	Magnetic anisotropy of Co^{II}W^Vferromagnet: single crystal and ab initio study. CrystEngComm, 2013, 15, 2378-2385.	1.3	14
93	Zeeman interaction and Jahn-Teller effect in the <math xmlns:mml="http://www.w3.org/1998/Math/MathML" <mathvariant="normal">^8</math> multiplet. Physical Review B, 2017, 96, .	1.1	14
94	Single Crystal Investigations Unravel the Magnetic Anisotropy of the "Square-In Square" Cr ₄ Dy ₄ SMM Coordination Cluster. Frontiers in Chemistry, 2019, 7, 6.	1.8	13
95	Toroidal versus centripetal arrangement of the magnetic moment in a Dy ₄ tetrahedron. Chemical Communications, 2022, 58, 1784-1787.	2.2	13
96	Understanding the magnetization blocking mechanism in N ₂ ˙-radical-bridged dilanthanide single-molecule magnets. Physical Chemistry Chemical Physics, 2021, 23, 10303-10310.	1.3	12
97	Mechanisms of Luminescence in Lanthanide Complexes: A Crucial Role of Metal-Ligand Covalency. Inorganic Chemistry, 2022, 61, 5972-5976.	1.9	11
98	<math xmlns:mml="http://www.w3.org/1998/Math/MathML" <mathvariant="normal">^8</math>-pseudospin states and the crystal field of cubic systems. Physical Review B, 2018, 98, .	1.1	10
99	Magnetization Dynamics on Isotope-Somorphonic Holmium Single-Molecule Magnets. Angewandte Chemie - International Edition, 2021, 60, 27282.	7.2	10
100	Probing the structural and magnetic properties of a new family of centrosymmetric dinuclear lanthanide complexes. RSC Advances, 2016, 6, 56668-56673.	1.7	9
101	Introduction to the electronic structure, luminescence, and magnetism of lanthanides. , 2018, , 1-58.		9
102	[Au^I(CN) ₂]-Armed [Fe^{III}]Fe^{II}] Square Complex Showing Unusual Spin-Crossover Behavior Due to a Symmetry-Breaking Phase Transition. Inorganic Chemistry, 2022, 61, 5855-5860.	1.9	9
103	Multiresponsive Spin Crossover Driven by Rotation of Tetraphenylborate Anion in an Iron(III) Complex. CCS Chemistry, 2021, 3, 453-459.	4.6	8
104	Manipulating the spin crossover behaviour in a series of cyanide-bridged {Fe ^{II} Fe ^{II} } molecular squares through NCE[˙] co-ligands. Dalton Transactions, 2022, 51, 5596-5602.	1.6	8
105	The Role of Radical Bridges in Polynuclear Single-Molecule Magnets. Chemistry - A European Journal, 2022, 28, e202200227.	1.7	8
106	Design of Fe^{III}-Ln^{III} binuclear complexes using compartmental ligands: synthesis, crystal structures, magnetic properties, and <i>ab initio</i> analysis. Journal of Materials Chemistry C, 2021, 9, 10912-10926.	2.7	7
107	Comparison of two field-induced Er^{III} single ion magnets. Dalton Transactions, 2019, 48, 15679-15686.	1.6	6
108	Magnetic Anisotropy in Divalent Lanthanide Compounds. Angewandte Chemie, 2020, 132, 12820-12824.	1.6	5

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109	Carbonate-free CoAl layered double hydroxides supercapacitors: Controlled precipitation via acid mediated decomplexation. <i>Applied Clay Science</i> , 2022, 224, 106519.	2.6	5
110	Dynamic Magnetic and Optical Insight into a High-Performance Pentagonal Bipyramidal Dy ^{III} Single-Molecule Magnet. <i>Chemistry - A European Journal</i> , 2017, 23, 5630-5630.	1.7	4
111	Towards understanding the magnetism of Os(^{IV}) complexes: an <i>ab initio</i> insight. <i>Dalton Transactions</i> , 2021, 50, 12537-12546.	1.6	3
112	Toroidal magnetic moments in Tb ₄ squares. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 784-791.	3.0	3
113	Correction to "Key Role of Frustration in Suppression of Magnetization Blocking in Single-Molecule Magnets". <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1678-1678.	2.1	2
114	Deriving the vibronic coupling constants of the cyclopentadienyl radical with density functional theory and GOWO. <i>Journal of Chemical Physics</i> , 2020, 153, 064303.	1.2	2
115	Exploring vibronic coupling in the benzene radical cation and anion with different levels of the <i>GW</i> approximation. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19054-19070.	1.3	1
116	Magnetization Dynamics on Isotope-Isomorphic Holmium Single-Molecule Magnets. <i>Angewandte Chemie</i> , 2021, 133, 27074-27074.	1.6	1
117	Stable Triarylmethyl Radicals and Cobalt(II) Ions Based 1D/2D Coordination Polymers. <i>Chemistry - A European Journal</i> , 2022, , .	1.7	1
118	Back Cover: A Non-sandwiched Macrocyclic Monolanthanide Single-Molecule Magnet: The Key Role of Axiality (<i>Chem. Eur. J.</i> 16/2011). <i>Chemistry - A European Journal</i> , 2011, 17, 4660-4660.	1.7	0
119	Innentitelbild: Magnetization Dynamics on Isotope-Isomorphic Holmium Single-Molecule Magnets (<i>Angew. Chem.</i> 52/2021). <i>Angewandte Chemie</i> , 2021, 133, 27074-27074.	1.6	0