

# David L Bryce

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/2389512/publications.pdf>

Version: 2024-02-01

188  
papers

6,189  
citations

66336

42  
h-index

106340

65  
g-index

202  
all docs

202  
docs citations

202  
times ranked

4879  
citing authors

#	ARTICLE	IF	CITATIONS
1	Definition of the chalcogen bond (IUPAC Recommendations 2019). <i>Pure and Applied Chemistry</i> , 2019, 91, 1889-1892.	1.9	322
2	Direct detection of CH/π interactions in proteins. <i>Nature Chemistry</i> , 2010, 2, 466-471.	13.6	247
3	Spin coupling tensors as determined by experiment and computational chemistry. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2002, 41, 233-304.	7.5	169
4	EFGShield – A program for parsing and summarizing the results of electric field gradient and nuclear magnetic shielding tensor calculations. <i>Canadian Journal of Chemistry</i> , 2007, 85, 496-505.	1.1	144
5	NMR crystallography: structure and properties of materials from solid-state nuclear magnetic resonance observables. <i>IUCr</i> , 2017, 4, 350-359.	2.2	115
6	A revised experimental absolute magnetic shielding scale for oxygen. <i>Journal of Chemical Physics</i> , 2002, 117, 10061-10066.	3.0	110
7	Potent inhibition of ice recrystallization by low molecular weight carbohydrate-based surfactants and hydrogelators. <i>Chemical Science</i> , 2012, 3, 1408.	7.4	102
8	Calcium-43 Chemical Shift Tensors as Probes of Calcium Binding Environments. Insight into the Structure of the Vaterite CaCO <sub>3</sub> Polymorph by <sup>43</sup> Ca Solid-State NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2008, 130, 9282-9292.	13.7	92
9	Zero Thermal Expansion in ZrMgMo <sub>3</sub> O <sub>12</sub> : NMR Crystallography Reveals Origins of Thermoelastic Properties. <i>Chemistry of Materials</i> , 2015, 27, 2633-2646.	6.7	90
10	NMR Investigations of Noncovalent Carbon Tetrel Bonds. Computational Assessment and Initial Experimental Observation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11891-11899.	2.5	88
11	High-Field Chlorine NMR Spectroscopy of Solid Organic Hydrochloride Salts: A Sensitive Probe of Hydrogen Bonding Environment. <i>Journal of Physical Chemistry A</i> , 2001, 105, 10413-10421.	2.5	84
12	QUEST – QUadrupolar EXact SOFTware: A fast graphical program for the exact simulation of NMR and NQR spectra for quadrupolar nuclei. <i>Solid State Nuclear Magnetic Resonance</i> , 2012, 45-46, 36-44.	2.3	77
13	Capsule Formation, Carboxylate Exchange, and DFT Exploration of Cadmium Cluster Metallocavitands: Highly Dynamic Supramolecules. <i>Journal of the American Chemical Society</i> , 2010, 132, 3893-3908.	13.7	75
14	Solid-state NMR spectroscopy of the quadrupolar halogens: chlorine-35/37, bromine-79/81, and iodine-127. <i>Magnetic Resonance in Chemistry</i> , 2006, 44, 409-450.	1.9	72
15	Halogen bonding as a supramolecular dynamics catalyst. <i>Nature Communications</i> , 2019, 10, 916.	12.8	72
16	Relaxation-Optimized NMR Spectroscopy of Methylene Groups in Proteins and Nucleic Acids. <i>Journal of the American Chemical Society</i> , 2004, 126, 10560-10570.	13.7	71
17	A high-field solid-state <sup>35/37</sup> Cl NMR and quantum chemical investigation of the chlorine quadrupolar and chemical shift tensors in amino acid hydrochlorides. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 6219.	2.8	71
18	A Solid-State <sup>11</sup> B NMR and Computational Study of Boron Electric Field Gradient and Chemical Shift Tensors in Boronic Acids and Boronic Esters. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5119-5131.	2.5	70

#	ARTICLE	IF	CITATIONS
19	Direct Investigation of Covalently Bound Chlorine in Organic Compounds by Solid-State <sup>35</sup> Cl NMR Spectroscopy and Exact Spectral Line-Shape Simulations. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 4227-4230.	13.8	69
20	Microwave Spectroscopy and Nuclear Magnetic Resonance Spectroscopy: What Is the Connection?. <i>Accounts of Chemical Research</i> , 2003, 36, 327-334.	15.6	67
21	Solid-state NMR of quadrupolar halogen nuclei. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2009, 55, 215-237.	7.5	67
22	Solid-State <sup>35/37</sup> Cl NMR Spectroscopy of Hydrochloride Salts of Amino Acids Implicated in Chloride Ion Transport Channel Selectivity: Opportunities at 900 MHz. <i>Journal of the American Chemical Society</i> , 2006, 128, 2121-2134.	13.7	64
23	Direct Investigation of Halogen Bonds by Solid-State Multinuclear Magnetic Resonance Spectroscopy and Molecular Orbital Analysis. <i>Journal of the American Chemical Society</i> , 2014, 136, 6929-6942.	13.7	64
24	Solid-State <sup>127</sup> I NMR and GIPAW DFT Study of Metal Iodides and Their Hydrates: Structure, Symmetry, and Higher-Order Quadrupole-Induced Effects. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10810-10823.	2.5	63
25	Correlation between <sup>13</sup> C chemical shifts and the halogen bonding environment in a series of solid para-diodotetrafluorobenzene complexes. <i>CrystEngComm</i> , 2013, 15, 3168.	2.6	63
26	Double Chalcogen Bonds: Crystal Engineering Stratagems via Diffraction and Multinuclear Solid-State Magnetic Resonance Spectroscopy. <i>Chemistry - A European Journal</i> , 2020, 26, 3275-3286.	3.3	61
27	Indirect Nuclear Spin-Spin Coupling Tensors in Diatomic Molecules: A Comparison of Results Obtained by Experiment and First Principles Calculations. <i>Journal of the American Chemical Society</i> , 2000, 122, 3197-3205.	13.7	60
28	Crystallographic structure refinement with quadrupolar nuclei: a combined solid-state NMR and GIPAW DFT example using MgBr <sub>2</sub> . <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 7120.	2.8	60
29	Alkaline Earth Chloride Hydrates: Chlorine Quadrupolar and Chemical Shift Tensors by Solid-State NMR Spectroscopy and Plane Wave Pseudopotential Calculations. <i>Chemistry - A European Journal</i> , 2007, 13, 4786-4796.	3.3	59
30	Signal enhancement in solid-state NMR of quadrupolar nuclei. <i>Solid State Nuclear Magnetic Resonance</i> , 2013, 51-52, 1-15.	2.3	58
31	Substituted 4,4'-Stilbenoid NCN-Pincer Platinum(II) Complexes. Luminescence and Tuning of the Electronic and NLO Properties and the Application in an OLED. <i>Organometallics</i> , 2008, 27, 1690-1701.	2.3	56
32	Calcium binding environments probed by <sup>43</sup> Ca NMR spectroscopy. <i>Dalton Transactions</i> , 2010, 39, 8593.	3.3	56
33	Periodic Trends in Indirect Nuclear Spin-Spin Coupling Tensors: Relativistic Density Functional Calculations for Interhalogen Diatomics. <i>Journal of the American Chemical Society</i> , 2002, 124, 4894-4900.	13.7	54
34	Multinuclear Magnetic Resonance Crystallographic Structure Refinement and Cross-Validation Using Experimental and Computed Electric Field Gradients: Application to Na <sub>2</sub> Al <sub>2</sub> B <sub>2</sub> O <sub>7</sub> . <i>Journal of Physical Chemistry C</i> , 2012, 116, 19472-19482.	3.1	52
35	Chlorine- <sup>35/37</sup> NMR Spectroscopy of Solid Amino Acid Hydrochlorides: Refinement of Hydrogen-Bonded Proton Positions Using Experiment and Theory. <i>Journal of Physical Chemistry B</i> , 2006, 110, 26461-26470.	2.6	47
36	Spying on the boron-boron triple bond using spin-spin coupling measured from <sup>11</sup> B solid-state NMR spectroscopy. <i>Chemical Science</i> , 2015, 6, 3378-3382.	7.4	47

#	ARTICLE	IF	CITATIONS
37	An <sup>17</sup> O NMR and Quantum Chemical Study of Monoclinic and Orthorhombic Polymorphs of Triphenylphosphine Oxide. <i>Inorganic Chemistry</i> , 2003, 42, 5085-5096.	4.0	46
38	A <sup>95</sup> Mo and <sup>13</sup> C solid-state NMR and relativistic DFT investigation of mesitylenetricarbonylmolybdenum(0) – a typical transition metal piano-stool complex. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 3591-3600.	2.8	45
39	Multinuclear Solid-State Magnetic Resonance and X-ray Diffraction Study of Some Thiocyanate and Selenocyanate Complexes Exhibiting Halogen Bonding. <i>Crystal Growth and Design</i> , 2011, 11, 4984-4995.	3.0	45
40	Weak Halogen Bonding in Solid Haloanilinium Halides Probed Directly via Chlorine-35, Bromine-81, and Iodine-127 NMR Spectroscopy. <i>Crystal Growth and Design</i> , 2012, 12, 1641-1653.	3.0	45
41	Mechanochemical Production of Halogen-Bonded Solids Featuring P=O=C Motifs and Characterization via X-ray Diffraction, Solid-State Multinuclear Magnetic Resonance, and Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27104-27117.	3.1	45
42	Liquid-crystal NMR structure of HIV TAR RNA bound to its SELEX RNA aptamer reveals the origins of the high stability of the complex. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 9210-9215.	7.1	44
43	Application of multinuclear magnetic resonance and gauge-including projector-augmented-wave calculations to the study of solid group 13 chlorides. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 6987.	2.8	44
44	<sup>35</sup> Cl Solid-State NMR and Computational Study of Chlorine Halogen Bond Donors in Single-Component Crystalline Chloronitriles. <i>Journal of Physical Chemistry C</i> , 2016, 120, 11121-11130.	3.1	44
45	Chapter 5 Chlorine, Bromine, and Iodine Solid-State NMR Spectroscopy. <i>Annual Reports on NMR Spectroscopy</i> , 2009, 66, 195-326.	1.5	43
46	Solid-State <sup>79/81</sup> Br NMR and Gauge-Including Projector-Augmented Wave Study of Structure, Symmetry, and Hydration State in Alkaline Earth Metal Bromides. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2102-2116.	2.5	43
47	Probing halogen bonds with solid-state NMR spectroscopy: observation and interpretation of <sup>77</sup> Se, <sup>31</sup> P coupling in halogen-bonded PtSeCl motifs. <i>CrystEngComm</i> , 2014, 16, 7285-7297.	2.6	43
48	Insight into the Structure of Silver Cyanide from <sup>13</sup> C and <sup>15</sup> N Solid-State NMR Spectroscopy. <i>Inorganic Chemistry</i> , 2002, 41, 4131-4138.	4.0	42
49	Chemical Shift Tensors of Protonated Base Carbons in Helical RNA and DNA from NMR Relaxation and Liquid Crystal Measurements. <i>Journal of the American Chemical Society</i> , 2006, 128, 11443-11454.	13.7	42
50	Cosublimation: A Rapid Route Toward Otherwise Inaccessible Halogen-Bonded Architectures. <i>Crystal Growth and Design</i> , 2018, 18, 6227-6238.	3.0	42
51	Multinuclear Solid-State Magnetic Resonance as a Sensitive Probe of Structural Changes upon the Occurrence of Halogen Bonding in Co-crystals. <i>Chemistry - A European Journal</i> , 2013, 19, 11949-11962.	3.3	41
52	Boron – boron coupling constants are unique probes of electronic structure: a solid-state NMR and molecular orbital study. <i>Chemical Science</i> , 2014, 5, 2428-2437.	7.4	40
53	Understanding the structural origin of crystalline phase transformations in nepheline (NaAlSi <sub>4</sub> ) – based glass-ceramics. <i>Journal of the American Ceramic Society</i> , 2017, 100, 2859-2878.	3.8	40
54	Sodium-23 Solid-State Nuclear Magnetic Resonance of Commercial Sodium Naproxen and its Solvates. <i>Journal of Pharmaceutical Sciences</i> , 2012, 101, 2930-2940.	3.3	39

#	ARTICLE	IF	CITATIONS
55	Ab initio characterization of through-space indirect nuclear spin-spin coupling tensors for fluorine-X (X=F, C, H) spin pairs. <i>Journal of Molecular Structure</i> , 2002, 602-603, 463-472.	3.6	37
56	Definitive solid-state <sup>185/187</sup> Re NMR spectral evidence for and analysis of the origin of high-order quadrupole-induced effects for I = 5/2. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 12413.	2.8	36
57	On the crystal structure of the vaterite polymorph of CaCO <sub>3</sub> : A calcium-43 solid-state NMR and computational assessment. <i>Solid State Nuclear Magnetic Resonance</i> , 2015, 65, 75-83.	2.3	36
58	A rare example of a phosphine as a halogen bond acceptor. <i>Chemical Communications</i> , 2018, 54, 11041-11043.	4.1	36
59	Effects of Secondary Anions on Proton Conduction in a Flexible Cationic Phosphonate Metal-Organic Framework. <i>Chemistry of Materials</i> , 2020, 32, 679-687.	6.7	36
60	Characterization of Tricoordinate Boron Chemical Shift Tensors: A Definitive High-Field Solid-State NMR Evidence for Anisotropic Boron Shielding. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3633-3640.	2.5	35
61	Comparing the Halogen Bond to the Hydrogen Bond by Solid-State NMR Spectroscopy: Anion Coordinated Dimers from $\pi$ - and $\sigma$ -iodoethynylpyridine Salts. <i>Chemistry - A European Journal</i> , 2018, 24, 11364-11376.	3.3	35
62	Measuring dipolar and $\langle i \rangle J \langle i \rangle$ coupling between quadrupolar nuclei using double-rotation NMR. <i>Journal of Chemical Physics</i> , 2013, 138, 174202.	3.0	34
63	<sup>13</sup> C and <sup>19</sup> F solid-state NMR and X-ray crystallographic study of halogen-bonded frameworks featuring nitrogen-containing heterocycles. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2017, 73, 157-167.	0.5	34
64	Recent advances in solid-state nuclear magnetic resonance spectroscopy of exotic nuclei. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2018, 109, 160-199.	7.5	34
65	Measurement of Five Dipolar Couplings from a Single 3D NMR Multiplet Applied to the Study of RNA Dynamics. <i>Journal of the American Chemical Society</i> , 2004, 126, 66-67.	13.7	33
66	Alkaline-Earth Metal Carboxylates Characterized by <sup>43</sup> Ca and <sup>87</sup> Sr Solid-State NMR: Impact of Metal-Amine Bonding. <i>Inorganic Chemistry</i> , 2014, 53, 552-561.	4.0	33
67	Direct investigation of chalcogen bonds by multinuclear solid-state magnetic resonance and vibrational spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 3817-3824.	2.8	33
68	Renaissance of the coordination chemistry of 2,4,6-tris(2-pyrimidyl)-1,3,5-triazine (TPymT). Part I: First crystal structure of a TPymT complex with a d-metal cation. <i>CrystEngComm</i> , 2013, 15, 10419.	2.6	32
69	The role of solid-state nuclear magnetic resonance in crystal engineering. <i>CrystEngComm</i> , 2016, 18, 5236-5252.	2.6	32
70	Solid-state NMR spectroscopy for the analysis of element-based non-covalent interactions. <i>Coordination Chemistry Reviews</i> , 2020, 411, 213237.	18.8	32
71	Symmetry-Amplified $\langle i \rangle J \langle i \rangle$ Splittings for Quadrupolar Spin Pairs: A Solid-State NMR Probe of Homoatomic Covalent Bonds. <i>Journal of the American Chemical Society</i> , 2013, 135, 12596-12599.	13.7	31
72	Prospects for <sup>207</sup> Pb solid-state NMR studies of lead tetrel bonds. <i>Faraday Discussions</i> , 2017, 203, 165-186.	3.2	31

#	ARTICLE	IF	CITATIONS
73	Solid-state <sup>11</sup> B and <sup>13</sup> C NMR, IR, and X-ray crystallographic characterization of selected arylboronic acids and their catechol cyclic esters. <i>Magnetic Resonance in Chemistry</i> , 2012, 50, 388-401.	1.9	30
74	Sterically Driven Olefin Metathesis: The Impact of Alkylidene Substitution on Catalyst Activity. <i>Organometallics</i> , 2016, 35, 691-698.	2.3	30
75	Measurement of Ribose Carbon Chemical Shift Tensors for A-form RNA by Liquid Crystal NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2005, 127, 7387-7396.	13.7	29
76	Application of Ultrahigh-Field <sup>59</sup> Co Solid-State NMR Spectroscopy in the Investigation of the 1,2-Polybutadiene Catalyst [Co(C <sub>8</sub> H <sub>13</sub> )(C <sub>4</sub> H <sub>6</sub> )]. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 3454-3457.	13.8	29
77	Application of Correlated Residual Dipolar Couplings to the Determination of the Molecular Alignment Tensor Magnitude of Oriented Proteins and Nucleic Acids. <i>Journal of Biomolecular NMR</i> , 2004, 28, 273-287.	2.8	28
78	Resolution-optimized NMR measurement of 1DCH, 1DCC and 2DCH residual dipolar couplings in nucleic acid bases. <i>Journal of Biomolecular NMR</i> , 2004, 30, 287-301.	2.8	28
79	A solid-state <sup>35/37</sup> Cl NMR study of a chloride ion receptor and a GIPAW-DFT study of chlorine NMR interaction tensors in organic hydrochlorides. <i>Canadian Journal of Chemistry</i> , 2011, 89, 822-834.	1.1	28
80	Interpretation of Indirect Nuclear Spin-Spin Coupling Tensors for Polyatomic Xenon Fluorides and Group 17 Fluorides: Results from Relativistic Density-Functional Calculations. <i>Inorganic Chemistry</i> , 2002, 41, 3091-3101.	4.0	27
81	Solid-State <sup>23</sup> Na NMR Study of Sodium Lariat Ether Receptors Exhibiting Cation-π Interactions. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13568-13577.	2.5	27
82	<sup>121/123</sup> Sb Nuclear Quadrupole Resonance Spectroscopy: Characterization of Non-Covalent Pnictogen Bonds and NQR Crystallography. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1030-1043.	2.5	27
83	Symmetry Properties of Indirect Nuclear Spin-Spin Coupling Tensors: First Principles Results for ClF <sub>3</sub> and OF <sub>2</sub> . <i>Journal of the American Chemical Society</i> , 2000, 122, 11236-11237.	13.7	26
84	Renaissance of the coordination chemistry of 2,4,6-tris(2-pyrimidyl)-1,3,5-triazine (TPymT). Part II: new insights into the reaction of TPymT with Pb(NO <sub>3</sub> ) <sub>2</sub> . <i>CrystEngComm</i> , 2014, 16, 3466-3469.	2.6	26
85	Halide ion recognition <i>via</i> chalcogen bonding in the solid state and in solution. Directionality and linearity. <i>CrystEngComm</i> , 2018, 20, 6406-6411.	2.6	26
86	Hyperfine Structure in the Rotational Spectrum of GaF: A Comparison of Experimental and Calculated Spin-Rotation and Electric Field Gradient Tensors. <i>Journal of Molecular Spectroscopy</i> , 2000, 204, 184-194.	1.2	25
87	Experimental and Theoretical Determination of Nucleic Acid Magnetic Susceptibility: Importance for the Study of Dynamics by Field-Induced Residual Dipolar Couplings. <i>Journal of the American Chemical Society</i> , 2004, 126, 10820-10821.	13.7	25
88	Solid-State NMR Study of Halogen-Bonded Adducts. <i>Topics in Current Chemistry</i> , 2014, 358, 183-203.	4.0	25
89	Hybrid Material Constructed from Hg(NCS) <sub>2</sub> and 2,4,6-Tris(2-pyrimidyl)-1,3,5-triazine (TPymT): Coordination of TPymT in a 2,2'-Bipyridine-Like Mode. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 441-446.	2.0	25
90	4,4'-Dipyridyl Dioxide-SbF <sub>3</sub> Cocrystal: Pnictogen Bond Prevails over Halogen and Hydrogen Bonds in Driving Self-Assembly. <i>Crystal Growth and Design</i> , 2020, 20, 916-922.	3.0	25



#	ARTICLE	IF	CITATIONS
91	NMR crystallography of sodium diphosphates: combining dipolar, shielding, quadrupolar, diffraction, and computational information. <i>CrystEngComm</i> , 2013, 15, 8727.	2.6	24
92	Recent Advances in Chlorine, Bromine, and Iodine Solid-State NMR Spectroscopy. <i>Annual Reports on NMR Spectroscopy</i> , 2015, , 115-162.	1.5	24
93	Interaction of 2,4,6-tris(2-pyrimidyl)-1,3,5-triazine (TPymT) with $\text{CoX}_2$ ( $X = \text{Cl}, \text{Br}$ ) in water: trapping of new self-assembled water-chloride/bromide clusters in a $[\text{Co}(\text{bpca})_2]^+\text{host}$ (bpca = bis(2-pyrimidylcarbonyl)amidate anion). <i>New Journal of Chemistry</i> , 2015, 39, 7147-7152.	2.8	23
94	Solid-state nuclear magnetic resonance and nuclear quadrupole resonance as complementary tools to study quadrupolar nuclei in solids. <i>Concepts in Magnetic Resonance Part A: Bridging Education and Research</i> , 2016, 45A, .	0.5	23
95	Chalcogen-Bonded Cocrystals of Substituted Pyridine N-Oxides and Chalcogenodiazoles: An X-ray Diffraction and Solid-State NMR Investigation. <i>Crystal Growth and Design</i> , 2020, 20, 7910-7920.	3.0	23
96	Ab Initio Calculations of NMR Parameters for Diatomic Molecules. An Exercise in Computational Chemistry. <i>Journal of Chemical Education</i> , 2001, 78, 124.	2.3	22
97	The first chromium-53 solid-state nuclear magnetic resonance spectra of diamagnetic chromium(0) and chromium(VI) compounds. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 5154-5157.	2.8	22
98	A Chelate-Stabilized Ruthenium( $\eta^5$ -pyrrolato) Complex: Resolving Ambiguities in Nuclearity and Coordination Geometry through $^1\text{H}$ PCSE and $^31\text{P}$ Solid-State NMR Studies. <i>Inorganic Chemistry</i> , 2006, 45, 10293-10299.	4.0	22
99	Postsynthetic modification of an imine-based microporous organic network. <i>Canadian Journal of Chemistry</i> , 2011, 89, 577-582.	1.1	22
100	Calcium-43 chemical shift and electric field gradient tensor interplay: a sensitive probe of structure, polymorphism, and hydration. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 13340-13359.	2.8	22
101	Halogen-bond driven self-assembly of triangular macrocycles. <i>New Journal of Chemistry</i> , 2018, 42, 10467-10471.	2.8	22
102	$^{79/81}\text{Br}$ nuclear quadrupole resonance spectroscopic characterization of halogen bonds in supramolecular assemblies. <i>Chemical Science</i> , 2018, 9, 4555-4561.	7.4	22
103	Mechanochemistry and cocrystallization of 3-iodoethynylbenzoic acid with nitrogen-containing heterocycles: concurrent halogen and hydrogen bonding. <i>New Journal of Chemistry</i> , 2018, 42, 10493-10501.	2.8	22
104	Modeling $^2\text{H}$ iso(N, N) in nucleic acid base pairs: ab initio characterization of the $^2\text{H}$ (N, N) tensor in the methyleneimine dimer as a function of hydrogen bond geometry. , 2001, 19, 371-375.		21
105	Residual dipolar coupling between quadrupolar nuclei under magic-angle spinning and double-rotation conditions. <i>Journal of Magnetic Resonance</i> , 2011, 213, 82-89.	2.1	21
106	Direct Characterization of Metal-Metal Bonds between Nuclei with Strong Quadrupolar Interactions via NMR Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 4049-4054.	4.6	21
107	Oxygen-17 NMR spectroscopy of water molecules in solid hydrates. <i>Canadian Journal of Chemistry</i> , 2016, 94, 189-197.	1.1	21
108	Short and Linear Intermolecular Tetrel Bonds to Tin. Cocrystal Engineering with Triphenyltin Chloride. <i>Crystal Growth and Design</i> , 2020, 20, 2027-2034.	3.0	21

#	ARTICLE	IF	CITATIONS
109	A multinuclear solid-state magnetic resonance and GIPAW DFT study of anhydrous calcium chloride and its hydrates. <i>Canadian Journal of Chemistry</i> , 2011, 89, 754-763.	1.1	20
110	A Combined Solid-State NMR and X-Ray Crystallography Study of the Bromide Ion Environments in Triphenylphosphonium Bromides. <i>Chemistry - A European Journal</i> , 2012, 18, 5748-5758.	3.3	20
111	NMR Crystallography. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2017, 73, 126-127.	0.5	20
112	A kinetic study of mechanochemical halogen bond formation by in situ <sup>31</sup> P solid-state NMR spectroscopy. <i>Chemical Communications</i> , 2017, 53, 9930-9933.	4.1	20
113	New frontiers for solid-state NMR across the periodic table: a snapshot of modern techniques and instrumentation. <i>Dalton Transactions</i> , 2019, 48, 8014-8020.	3.3	20
114	Beryllium-9 NMR Study of Solid Bis(2,4-pentanedionato-O,O <sup>2-</sup> )beryllium and Theoretical Studies of <sup>9</sup> Be Electric Field Gradient and Chemical Shielding Tensors. First Evidence for Anisotropic Beryllium Shielding. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7364-7372.	2.5	19
115	A Solid-State Multinuclear Magnetic Resonance Investigation of Hexamethylborazine. <i>Journal of Physical Chemistry A</i> , 2003, 107, 726-735.	2.5	19
116	Theoretical study of homonuclear J coupling between quadrupolar spins: Single-crystal, DOR, and J-resolved NMR. <i>Journal of Magnetic Resonance</i> , 2014, 242, 23-32.	2.1	19
117	Structure and solubility behaviour of zinc containing phosphate glasses. <i>Journal of Materials Chemistry B</i> , 2015, 3, 8842-8855.	5.8	19
118	<sup>23</sup> Na double-rotation NMR of sodium nucleotides leads to the discovery of a new dCMP hendecahydrate. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 4677.	2.8	18
119	High sensitivity and resolution in <sup>43</sup> Ca solid-state NMR experiments. <i>Canadian Journal of Chemistry</i> , 2015, 93, 799-807.	1.1	18
120	Solid-state <sup>185/187</sup> Re NMR and GIPAW DFT study of perrhenates and Re <sub>2</sub> (CO) <sub>10</sub> : chemical shift anisotropy, NMR crystallography, and a metal-metal bond. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10118-10134.	2.8	18
121	From discrete molecule, to polymer, to MOF: mapping the coordination chemistry of Cd <sup>II</sup> using <sup>113</sup> Cd solid-state NMR. <i>Chemical Communications</i> , 2016, 52, 10680-10683.	4.1	18
122	Using <sup>69/71</sup> Ga solid-state NMR and <sup>127</sup> I NQR as probes to elucidate the composition of $\alpha$ -Ga <sub>2</sub> Polyhedron, 2012, 35, 96-100.	2.2	17
123	Observation of CH <sub>2</sub> ... $\pi$ Interactions between Methyl and Carbonyl Groups in Proteins. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 7564-7567.	13.8	17
124	1,3,5-Tri(iodoethynyl)-2,4,6-trifluorobenzene: halogen-bonded frameworks and NMR spectroscopic analysis. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 153-162.	1.1	17
125	Computational approaches and sigma-hole interactions: general discussion. <i>Faraday Discussions</i> , 2017, 203, 131-163.	3.2	17
126	Rapid Identification of Halogen Bonds in Co <sup>II</sup> Crystalline Powders via <sup>127</sup> I Nuclear Quadrupole Resonance Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 13479-13485.	13.8	17



#	ARTICLE	IF	CITATIONS
127	Single-Crystal NMR Characterization of Halogen Bonds. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6194-6209.	2.5	17
128	Recent Advances in <sup>11</sup> B Solid-State Nuclear Magnetic Resonance Spectroscopy of Crystalline Solids. <i>Annual Reports on NMR Spectroscopy</i> , 2018, , 213-279.	1.5	16
129	<sup>K-39</sup> Quadrupolar and Chemical Shift Tensors for Organic Potassium Complexes and Diatomic Molecules. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12859-12863.	2.5	15
130	NMR line shapes from AB spin systems in solids – The role of antisymmetric spin–spin coupling. <i>Canadian Journal of Chemistry</i> , 2009, 87, 1338-1351.	1.1	15
131	First structural evidence for multiple alkali metals between sandwich decks in a metallocene. <i>Dalton Transactions</i> , 2012, 41, 8060.	3.3	15
132	Intercalation of Coordinatively Unsaturated Fe <sup>III</sup> Ion within Interpenetrated Metal–Organic Framework MOF-5. <i>Chemistry - A European Journal</i> , 2016, 22, 7711-7715.	3.3	15
133	<sup>11</sup> B Solid-State NMR Interaction Tensors of Linear Two-Coordinate Boron: The Dimethylborinium Cation. <i>Inorganic Chemistry</i> , 2015, 54, 11889-11896.	4.0	14
134	New Experimental Insight into the Nature of Metal–Metal Bonds in Digallium Compounds: <i>J</i> Coupling between Quadrupolar Nuclei. <i>Chemistry - A European Journal</i> , 2016, 22, 9565-9573.	3.3	14
135	Dynamic Disorder and Electronic Structures of Electron-Precise Dianionic Diboranes: Insights from Solid-State Multinuclear Magnetic Resonance Spectroscopy. <i>Journal of the American Chemical Society</i> , 2017, 139, 8200-8211.	13.7	14
136	Enhanced spectral resolution in RNA HCP spectra for measurement of <sup>3</sup> J <sub>C2</sub> and <sup>3</sup> J <sub>C4</sub> couplings and <sup>31</sup> P chemical shift changes upon weak alignment. <i>Journal of Biomolecular NMR</i> , 2004, 30, 61-70.	2.8	13
137	Measurement of <sup>1</sup> J( <sup>199</sup> Hg, <sup>31</sup> P) in [HgPCy <sub>3</sub> (OAc) <sub>2</sub> ] <sub>2</sub> and relativistic ZORA DFT investigations of mercury–phosphorus coupling tensors. <i>Solid State Nuclear Magnetic Resonance</i> , 2009, 36, 182-191.	2.3	13
138	<sup>23</sup> Na magic-angle spinning and double-rotation NMR study of solid forms of sodium valproate. <i>Canadian Journal of Chemistry</i> , 2014, 92, 9-15.	1.1	13
139	Multinuclear Solid-State Magnetic Resonance Study of In <sup>+</sup> and Ag <sup>+</sup> in Neutral Weakly Coordinating Environments. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 3078-3084.	4.6	12
140	Insight into Magnesium Coordination Environments in Benzoate and Salicylate Complexes through <sup>25</sup> Mg Solid-State NMR Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6561-6570.	2.5	12
141	Field-stepped ultra-wideline NMR at up to 36 T: On the inequivalence between field and frequency stepping. <i>Magnetic Resonance in Chemistry</i> , 2021, 59, 951-960.	1.9	12
142	Recent advances in NMR crystallography and polymorphism. <i>Annual Reports on NMR Spectroscopy</i> , 2021, 102, 1-80.	1.5	11
143	Experimental <sup>13</sup> C and <sup>1</sup> H Solid-State NMR Response in Weakly Tetrel-Bonded Methyl Groups. <i>Journal of Physical Chemistry C</i> , 2021, 125, 2111-2123.	3.1	10
144	NMR Response of the Tetrel Bond Donor. <i>Journal of Physical Chemistry C</i> , 2022, 126, 851-865.	3.1	10

#	ARTICLE	IF	CITATIONS
145	Combining oximes with azides to create a novel 1-D [NaCo <sup>III</sup> ] <sub>2</sub> system: synthesis, structure and solid-state NMR. Dalton Transactions, 2010, 39, 1504-1510.	3.3	9
146	Solid-State NMR Studies of Halogen Bonding. , 2016, , 1-18.		9
147	Dipolar-Chemical Shift and Rotational Resonance <sup>13</sup> C NMR Studies of the Carboxylate Methylene Carbon Spin Pair in Solid Phenylacetic Acid and Potassium Hydrogen Bisphenylacetate. Journal of Physical Chemistry A, 2000, 104, 7700-7710.	2.5	8
148	Structural Insights from <sup>59</sup> Co Solid-State NMR Experiments on Organocobalt(II) Catalysts. ChemPhysChem, 2018, 19, 227-236.	2.1	8
149	Mechanochemical Preparations of Anion Coordinated Architectures Based on 3-Ethynylpyridine and 3-Ethynylbenzoic Acid. ChemistryOpen, 2019, 8, 1328-1336.	1.9	8
150	Evaluation of the influence of anisotropic indirect nuclear spin-spin coupling tensors on effective residual dipolar couplings for model peptides. Journal of Biomolecular NMR, 2003, 25, 73-78.	2.8	7
151	A computational investigation of J couplings involving <sup>27</sup> Al, <sup>17</sup> O, and <sup>31</sup> P. Magnetic Resonance in Chemistry, 2010, 48, S69-S75.	1.9	7
152	Multinuclear solid-state magnetic resonance study of oxo-bridged dinickel and quadruply-bonded dimolybdenum carboxylate clusters. Solid State Nuclear Magnetic Resonance, 2017, 84, 20-27.	2.3	7
153	Structural and Crystallographic Information from <sup>61</sup> Ni Solid-State NMR Spectroscopy: Diamagnetic Nickel Compounds. Inorganic Chemistry, 2017, 56, 9996-10006.	4.0	7
154	On the importance of accurate nuclear quadrupole moments in <sup>31</sup> P NMR crystallography. Magnetic Resonance in Chemistry, 2019, 57, 265-267.	1.9	6
155	SCFit: Software for single-crystal NMR analysis. Free vs constrained fitting. Solid State Nuclear Magnetic Resonance, 2019, 102, 53-62.	2.3	6
156	Recent advances in chlorine, bromine, and iodine solid-state NMR spectroscopy. Annual Reports on NMR Spectroscopy, 2020, 100, 97-152.	1.5	6
157	Observation of CH...N Interactions between Methyl and Carbonyl Groups in Proteins. Angewandte Chemie, 2017, 129, 7672-7675.	2.0	5
158	The halogen bond in solution: general discussion. Faraday Discussions, 2017, 203, 347-370.	3.2	5
159	Linear dicoordinate beryllium: a <sup>9</sup> Be solid-state NMR study of a discrete zero-valent s-block beryllium complex. Canadian Journal of Chemistry, 2018, 96, 646-652.	1.1	5
160	π-Complexes of Diborynes with Main Group Atoms. Chemistry - an Asian Journal, 2020, 15, 1553-1557.	3.3	5
161	Predictability of Chalcogen-Bond-Driven Crystal Engineering: An X-ray Diffraction and Selenium-77 Solid-State NMR Investigation of Benzylic Selenocyanate Cocrystals. ACS Organic & Inorganic Au, 2022, 2, 252-260.	4.0	5
162	Stoichiometric halogen-bonded cocrystals: a case study of 1,4-diodotetrafluorobenzene and 3-nitropyridine. Canadian Journal of Chemistry, 2022, 100, 245-251.	1.1	4

#	ARTICLE	IF	CITATIONS
163	Solid-State NMR, Rotational Resonance. , 1999, , 2136-2144.		3
164	Removal of sidebands in double-rotation NMR in real time. Journal of Magnetic Resonance, 2011, 211, 234-239.	2.1	3
165	Rapid Identification of Halogen Bonds in Coâ€Crystalline Powders via 127 I Nuclear Quadrupole Resonance Spectroscopy. Angewandte Chemie, 2019, 131, 13613-13619.	2.0	3
166	A ZORA-DFT and NLMO study of the one-bond fluorineâ€X indirect nuclear spin-spin coupling tensors for various VSEPR geometries. Canadian Journal of Chemistry, 2011, 89, 789-802.	1.1	2
167	Beyond the halogen bond: general discussion. Faraday Discussions, 2017, 203, 227-244.	3.2	2
168	Solid-state chemistry and applications: general discussion. Faraday Discussions, 2017, 203, 459-483.	3.2	2
169	Crystal structure of tetrabutylammonium bromideâ€1,2-diiodo-3,4,5,6-tetrafluorobenzeneâ€dichloromethane (2/2/1). Acta Crystallographica Section E: Crystallographic Communications, 2015, 71, o286-o287.	0.5	2
170	To what extent do bond length and angle govern the 13C and 1H NMR response to weak CHâ€O hydrogen bonds? A case study of caffeine and theophylline cocrystals. Solid State Nuclear Magnetic Resonance, 2022, 119, 101795.	2.3	2
171	Spinâ€spin coupling constants in homonuclear polynitrogen species. Physical Chemistry Chemical Physics, 2006, 8, 3379-3382.	2.8	1
172	Solid-State NMR at the University of Ottawa. Canadian Journal of Chemistry, 2015, 93, 485-491.	1.1	1
173	3-(1,2,2-Triiodoethenyl)benzoic acid. IUCrData, 2018, 3, .	0.3	1
174	Assessment of halogen-bond induced cocrystallization of 1,3,5-trihalo-2,4,6-trifluorobenzenes with 2,3,5,6-Tetramethylpyrazine. Results in Chemistry, 2022, 4, 100336.	2.0	1
175	Solid-state multinuclear magnetic resonance and X-ray crystallographic investigation of the phosphorus...iodine halogen bond in a bis(dicyclohexylphenylphosphine)(1,6-diiodoperfluorohexane) cocrystal. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 557-563.	1.1	1
176	Solid-state NMR of quadrupolar nuclei: Selected new methods and applications. Annual Reports on NMR Spectroscopy, 2022, , .	1.5	1
177	Solid State NMR, Rotational Resonance*. , 1999, , 2595-2603.		0
178	Microwave Spectroscopy and Nuclear Magnetic Resonance Spectroscopy â€” What Is the Connection?. ChemInform, 2003, 34, no.	0.0	0
179	Crystal structure of tetraethylammonium chloride 3,4,5,6-tetrafluoro-1,2-diiodobenzene. Acta Crystallographica Section E: Crystallographic Communications, 2015, 71, o319-o320.	0.5	0
180	Editorial - A dynamic journal. Solid State Nuclear Magnetic Resonance, 2018, 96, A1.	2.3	0

#	ARTICLE	IF	CITATIONS
181	Editorial: Special Issue on Emerging Frontiers in Dynamic Nuclear Polarization NMR. Solid State Nuclear Magnetic Resonance, 2019, 102, 1.	2.3	0
182	Mechanochemical Preparations of Anion Coordinated Architectures Based on 3-iodoethynylpyridine and 3-iodoethynylbenzoic Acid. ChemistryOpen, 2019, 8, 1327-1327.	1.9	0
183	Frontispiece: Double Chalcogen Bonds: Crystal Engineering Stratagems via Diffraction and Multinuclear Solid-State Magnetic Resonance Spectroscopy. Chemistry - A European Journal, 2020, 26, .	3.3	0
184	Editorial: Industrial applications of solid-state NMR. Solid State Nuclear Magnetic Resonance, 2020, 107, 101667.	2.3	0
185	One Ball Tips the Balance toward Three-Component Borromean Ring Systems. Chem, 2021, 7, 9-11.	11.7	0
186	Solid State NMR, Rotational Resonance. , 2017, , 106-113.		0
187	Solid-State NMR Studies of Halogen Bonding. , 2018, , 1031-1047.		0
188	NMR Crystallography of Monovalent Cations in Inorganic Matrices: Na <sup>+</sup> Siting and the Local Structure of Na <sup>+</sup> Sites in Ferrierites. Journal of Physical Chemistry C, 0, , .	3.1	0