Paul Hodgkinson

List of Publications by Year
in descending order

100	3,878	126708	143772
papers	citations	33 h-index	57 g-index

113	113	113	3175
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Homonuclear dipolar decoupling in solid-state NMR using continuous phase modulation. Chemical Physics Letters, 2000, 319, 253-260.	1.2	282
2	Chemical shift computations on a crystallographic basis: some reflections and comments. Magnetic Resonance in Chemistry, 2007, 45, S174-S186.	1.1	197
3	Origins of linewidth in H1 magic-angle spinning NMR. Journal of Chemical Physics, 2006, 125, 144508.	1.2	121
4	Spectroscopic and Structural Characterization of the CyNHC Adduct of B₂pin₂ in Solution and in the Solid State. Journal of Organic Chemistry, 2012, 77, 785-789.	1.7	121
5	The reliability of the determination of tensor parameters by solid-state nuclear magnetic resonance. Journal of Chemical Physics, 1997, 107, 4808-4816.	1.2	106
6	Optimal Sampling Strategies for the Measurement of Spinâ€“Spin Relaxation Times. Journal of Magnetic Resonance Series B, 1996, 113, 25-34.	1.6	104
7	Transverse Dephasing Optimized Solid-State NMR Spectroscopy. Journal of the American Chemical Society, 2003, 125, 13938-13939.	6.6	104
8	A Novel Detectionâ€“Estimation Scheme for Noisy NMR Signals: Applications to Delayed Acquisition Data. Journal of Magnetic Resonance, 1997, 128, 30-41.	1.2	102
9	Heteronuclear decoupling in the NMR of solids. Progress in Nuclear Magnetic Resonance Spectroscopy, 2005, 46, 197-222.	3.9	102
10	Numerical simulation of solid-state NMR experiments. Progress in Nuclear Magnetic Resonance Spectroscopy, 2000, 36, 201-239.	3.9	100
11	NMR crystallography of molecular organics. Progress in Nuclear Magnetic Resonance Spectroscopy, 2020, 118-119, 10-53.	3.9	95
12	A molecular dynamics study of the effects of fast molecular motions on solid-state NMR parameters. CrystEngComm, 2013, 15, 8705.	1.3	77
13	Computation and NMR crystallography of terbutaline sulfate. Magnetic Resonance in Chemistry, 2010, 48, S103-S112.	1.1	76
14	The Accuracy of Distance Measurements in Solid-State NMR. Journal of Magnetic Resonance, 1999, 139, 46-59.	1.2	67
15	Structural Study of Polymorphs and Solvates of Finasteride. Journal of Pharmaceutical Sciences, 2007, 96, 1380-1397.	1.6	65
16	Improved heteronuclear decoupling schemes for solid-state magic angle spinning NMR by direct spectral optimization. Chemical Physics Letters, 2003, 376, 259-267.	1.2	63
17	Characterisation of indomethacin and nifedipine using variable-temperature solid-state NMR. Magnetic Resonance in Chemistry, 2005, 43, 881-892.	1.1	61
18	Quantifying hydrogen-bonding strength: the measurement of 2hJNN couplings in self-assembled guanosines by solid-state 15N spin-echo MAS NMR. Physical Chemistry Chemical Physics, 2007, 9, 3416.	1.3	60

#	Article	IF	Citations
19	Understanding two-pulse phase-modulated decoupling in solid-state NMR. Journal of Chemical Physics, 2009, 130, 114510.	1.2	60
20	Visualization and processing of computed solid-state NMR parameters: MagresView and MagresPython. Solid State Nuclear Magnetic Resonance, 2016, 78, 64-70.	1.5	57
21	Quantification of bambuterol hydrochloride in a formulated product using solid-state NMR. Journal of Pharmaceutical and Biomedical Analysis, 2005, 38, 858-864.	1.4	56
22	Temperature Dependence of NMR Parameters Calculated from Path Integral Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2016, 12, 968-973.	2.3	54
23	Hydrogen Bonding and Dynamic Behaviour in Crystals and Polymorphs of Dicarboxylicâ€“Diamine Adducts: A Comparison between NMR Parameters and X-ray Diffraction Studies. Chemistry - A European Journal, 2005, 11, 7461-7471.	1.7	52
24	Effects of Quantum Nuclear Delocalisation on NMR Parameters from Path Integral Molecular Dynamics. Chemistry - A European Journal, 2014, 20, 2201-2207.	1.7	52
25	Quantification of homonuclear dipolar coupling networks from magic-angle spinning1H NMR. Molecular Physics, 2006, 104, 293-304.	0.8	51
26	Furosemide's one little hydrogen atom: NMR crystallography structure verification of powdered molecular organics. Chemical Communications, 2016, 52, 6685-6688.	2.2	49
27	Improved Proton Decoupling in NMR Spectroscopy of Crystalline Solids Using the S PINAL -64 Sequence. Monatshefte FÃ¼r Chemie, 2002, 133, 1549-1554.	0.9	45
28	High-Resolution 1H NMR Spectroscopy of Solids. Annual Reports on NMR Spectroscopy, 2011, 72, 185-223.	0.7	43
29	Heteronuclear decoupling in NMR of Liquid Crystals using continuous phase modulation. Chemical Physics Letters, 2003, 368, 511-522.	1.2	42
30	NMR studies of exchange between triazine rotamers. Magnetic Resonance in Chemistry, 2000, 38, 504-511.	1.1	39
31	Combining insights from solid-state NMR and first principles calculation: applications to the 19F NMR of octafluoronaphthalene. Physical Chemistry Chemical Physics, 2007, 9, 2389.	1.3	39
32	A furosemideâ€“isonicotinamide cocrystal: an investigation of properties and extensive structural disorder. CrystEngComm, 2015, 17, 6707-6715.	1.3	38
33	Characterization of Polymorphs and Solvates of Terbutaline Sulfate. Crystal Growth and Design, 2008, 8, 80-90.	1.4	36
34	Towards homonuclear J solid-state NMR correlation experiments for half-integer quadrupolar nuclei: experimental and simulated 11B MAS spin-echo dephasing and calculated 2JBB coupling constants for lithium diborate. Physical Chemistry Chemical Physics, 2011, 13, 5778.	1.3	34
35	Improving Confidence in Crystal Structure Solutions Using NMR Crystallography: The Case of Î²-Piroxicam. Crystal Growth and Design, 2018, 18, 3339-3351.	1.4	34
36	Characterization of Oxygen Dynamics in ZrW2O8. Journal of the American Chemical Society, 2005, 127, 15175-15181.	6.6	33

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37	Simulation of extended periodic systems of nuclear spins. Chemical Physics Letters, 2000, 326, 515-522.	1.2	32
38	Using17O solid-state NMR and first principles calculation to characterise structure and dynamics in inorganic framework materials. Magnetic Resonance in Chemistry, 2007, 45, S144-S155.	1.1	31
39	Experimental observation of periodic quasi-equilibria in solid-state NMR. Chemical Physics Letters, 1999, 308, 381-389.	1.2	30
40	Characterization of Two Distinct Amorphous Forms of Valsartan by Solid-State NMR. Molecular Pharmaceutics, 2016, 13, 211-222.	2.3	30
41	Assignment and Measurement of Deuterium Quadrupolar Couplings in Liquid Crystals by Deuteriumâ^'Carbon NMR Correlation Spectroscopy. Journal of Physical Chemistry B, 1998, 102, 3718-3723.	1.2	28
42	The nature of oxygen exchange in ZrW2O8 revealed by two-dimensional solid-state 17O NMR. Chemical Communications, 2004, , 392.	2.2	28
43	Structure and physicochemical characterization of a naproxenâ€“picolinamide cocrystal. Acta Crystallographica Section C, Structural Chemistry, 2017, 73, 168-175.	0.2	28
44	Perspective: Current advances in solid-state NMR spectroscopy. Journal of Chemical Physics, 2018, 149, 040901.	1.2	28
45	Proton transfer in guanineâ€“cytosine base pair analogues studied by NMR spectroscopy and PIMD simulations. Faraday Discussions, 2018, 212, 331-344.	1.6	28
46	Structures and Phase Transitions in (MoO₂)₂P₂O₇. Inorganic Chemistry, 2010, 49, 2290-2301.	1.9	27
47	Solid-state NMR studies of nucleic acid components. RSC Advances, 2015, 5, 12300-12310.	1.7	27
48	Elucidation of Structure and Dynamics in Solid Octafluoronaphthalene from Combined NMR, Diffraction, And Molecular Dynamics Studies. Journal of the American Chemical Society, 2010, 132, 5179-5185.	6.6	26
49	NMR characterisation of dynamics in solvates and desolvates of formoterol fumarate. Physical Chemistry Chemical Physics, 2013, 15, 6422.	1.3	25
50	Testing the limits of NMR crystallography: the case of caffeineâ€“citric acid hydrate. CrystEngComm, 2016, 18, 6700-6707.	1.3	25
51	Characterising the role of water in sildenafil citrate by NMR crystallography. CrystEngComm, 2016, 18, 1054-1063.	1.3	25
52	Insights into homonuclear decoupling from efficient numerical simulation: Techniques and examples. Journal of Magnetic Resonance, 2008, 192, 183-196.	1.2	23
53	Deuteriumâ^'Carbon NMR Correlation Spectroscopy in Oriented Materials. Journal of the American Chemical Society, 1997, 119, 12000-12001.	6.6	22
54	Computation of magnetic shielding to simultaneously validate a crystal structure and assign a solid-state NMR spectrum. Journal of Molecular Structure, 2012, 1015, 192-201.	1.8	22

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55	Bisoprolol and Bisoprolol-Valsartan Compatibility Studied by Differential Scanning Calorimetry, Nuclear Magnetic Resonance and X-Ray Powder Diffractometry. Pharmaceutical Research, 2015, 32, 414-429.	1.7	22
56	Shape-selective crystallisation of fluxional carbon cages. Chemical Science, 2018, 9, 8631-8636.	3.7	22
57	Deuterium to carbon cross-polarization in liquid crystals. Journal of Chemical Physics, 1998, 109, 1873-1884.	1.2	21
58	Solid-state109Ag CP/MAS NMR spectroscopy of some diammine silver(I) complexes. Magnetic Resonance in Chemistry, 2004, 42, 819-826.	1.1	21
59	Solid-state NMR studies of some tin(II) compounds. Solid State Nuclear Magnetic Resonance, 2004, 26, 160-171.	1.5	21
60	A Multi-Technique Approach to the Study of Structural Stability and Desolvation of Two Unusual Channel Hydrate Solvates of Finasteride. Journal of Pharmaceutical Sciences, 2012, 101, 176-186.	1.6	21
61	Well-Tempered Metadynamics as a Tool for Characterizing Multi-Component, Crystalline Molecular Machines. Journal of Physical Chemistry B, 2013, 117, 12286-12295.	1.2	21
62	Na⁺ mobility in sodium strontium silicate fast ion conductors. Chemical Communications, 2015, 51, 17163-17165.	2.2	21
63	Solid-state NMR and computational investigation of solvent molecule arrangement and dynamics in isostructural solvates of droperidol. Solid State Nuclear Magnetic Resonance, 2015, 65, 12-20.	1.5	21
64	Quasi equilibria in solid-state NMR. Chemical Physics Letters, 1998, 293, 110-118.	1.2	20
65	Resonance-assisted stabilisation of hydrogen bonds probed by NMR spectroscopy and path integral molecular dynamics. Chemical Communications, 2015, 51, 13986-13989.	2.2	20
66	Exploring Systematic Discrepancies in DFT Calculations of Chlorine Nuclear Quadrupole Couplings. Journal of Physical Chemistry A, 2017, 121, 4103-4113.	1.1	19
67	Resolving alternative organic crystal structures using density functional theory and NMR chemical shifts. Chemical Science, 2020, 11, 2987-2992.	3.7	18
68	Structural Properties of Carboxylic Acid Dimers Confined within the Urea Tunnel Structure: An MD Simulation Study. Journal of Physical Chemistry B, 2011, 115, 2791-2800.	1.2	16
69	Cross-polarization efficiency in INS systems using adiabatic RF sweeps. Journal of Chemical Physics, 1997, 107, 8742-8751.	1.2	15
70	On the orientational dependence of resolution in1H solid-state NMR, and its role in MAS, CRAMPS and delayed-acquisition experiments. Magnetic Resonance in Chemistry, 2007, 45, S93-S100.	1.1	15
71	Line-splitting and broadening effects from 19F in the 13CNMR of liquid crystals and solids. Chemical Physics Letters, 2001, 344, 68-74.	1.2	14
72	Synthesis and NMR studies of 17O enriched AM2O8 phases. Solid State Sciences, 2005, 7, 819-826.	1.5	14

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73	Structural characterisation of two pharmaceutically important steroids by solid-state NMR. New Journal of Chemistry, 2008, 32, 1796.	1.4	14
74	NMR characterisation of structure in solvates and polymorphs of formoterol fumarate. Magnetic Resonance in Chemistry, 2012, 50, 680-690.	1.1	14
75	Towards Accurate Predictions of Proton NMR Spectroscopic Parameters in Molecular Solids. ChemPhysChem, 2020, 21, 2075-2083.	1.0	14
76	Use of rotary echoes in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si8.gif" display="inline" overflow="scroll"><mml:mrow><mml:msup><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msup><mml:mi mathvariant="normal">H</mml:mi></mml:mrow></mml:math> magic-angle spinning NMR for the quantitative study of molecular dynamics. Chemical Physics Letters, 2009, 475, 58-63.	1.2	12
77	Dynamics of water molecules and sodium ions in solid hydrates of nucleotides. CrystEngComm, 2014, 16, 6756-6764.	1.3	12
78	Synthesis and structural characterization of cocrystals of isoniazid and cinnamic acid derivatives. Journal of Molecular Structure, 2020, 1219, 128621.	1.8	12
79	Selective Data Acquisition in NMR. The Quantification of Anti-phase Scalar Couplings. Journal of Magnetic Resonance Series A, 1996, 120, 18-30.	1.6	11
80	Application of Maximum Entropy Methods to Three-Dimensional NMR Spectroscopy. Journal of Magnetic Resonance Series B, 1993, 101, 218-222.	1.6	10
81	Sampling and the quantification of NMR data. Advances in Magnetic and Optical Resonance, 1997, 20, 187-244.	1.7	10
82	Resolution of 13Câ€“19F interactions in the 13C NMR of spinning solids and liquid crystals. Journal of Magnetic Resonance, 2004, 168, 124-131.	1.2	9
83	Solid-state NMR spectroscopy. Physical Chemistry Chemical Physics, 2009, 11, 6875.	1.3	9
84	Paramagnetic solid-state NMR assignment and novel chemical conversion of the aldehyde group to dihydrogen ortho ester and hemiacetal moieties in copper(<scp>ii</scp>)- and cobalt(<scp>ii</scp>)-pyridinecarboxaldehyde complexes. RSC Advances, 2021, 11, 20216-20231.	1.7	9
85	Interference of homonuclear decoupling and exchange in the solid-state NMR of perfluorocyclohexane. Journal of Magnetic Resonance, 2003, 161, 234-241.	1.2	7
86	Unexpected effects of third-order cross-terms in heteronuclear spin systems under simultaneous radio-frequency irradiation and magic-angle spinning NMR. Journal of Chemical Physics, 2012, 136, 084503.	1.2	7
87	Rationalising Heteronuclear Decoupling in Refocussing Applications of Solidâ€State NMR Spectroscopy. ChemPhysChem, 2017, 18, 394-405.	1.0	7
88	NMR studies of31P,â€‰1H spin pairs in solid tin(II) phosphite and tin(II) hydrogen phosphate. Molecular Physics, 2004, 102, 877-882.	0.8	6
89	Quantitative analysis of 17O exchange and relaxation data: Application to zirconium tungstate. Solid State Nuclear Magnetic Resonance, 2006, 30, 98-105.	1.5	6
90	Tailored Acquisition in Chemical-Shift Imaging. Journal of Magnetic Resonance Series B, 1994, 105, 256-259.	1.6	5

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91	Optimizing Spatially Localized NMR. Journal of Magnetic Resonance Series B, 1995, 106, 261-269.	1.6	5
92	Simulating spin dynamics in organic solids under heteronuclear decoupling. Solid State Nuclear Magnetic Resonance, 2015, 70, 28-37.	1.5	5
93	Characterization of crystalline and amorphous forms of irbesartan by multi-nuclear solid-state NMR. Solid State Nuclear Magnetic Resonance, 2022, 118, 101783.	1.5	5
94	Stray-field NMR diffusion q -space diffraction imaging of monodisperse coarsening foams. Journal of Colloid and Interface Science, 2016, 476, 20-28.	5.0	4
95	Improved Proton Decoupling in NMR Spectroscopy of Crystalline Solids Using the Spinal-64 Sequence. , 2002, , 69-74.		3
96	Resolving alternative structure determinations of indapamide using ¹³C solid-state NMR. Chemical Communications, 2022, 58, 4767-4770.	2.2	2
97	A study of the dynamics and structure of the dielectric anomaly within the molecular solid TEA(TCNQ)₂. Physical Chemistry Chemical Physics, 2022, 24, 7481-7492.	1.3	2
98	The Nature of Oxygen Exchange in ZrW2O8 Revealed by Two-Dimensional Solid-State17O NMR.. ChemInform, 2004, 35, no.	0.1	1
99	Perspectives: In crystallography we trust. C&EN Global Enterprise, 2016, 94, 30-31.	0.0	1
100	Characterization of Oxygen Dynamics in ZrW2O8.. ChemInform, 2006, 37, no.	0.1	0