Paul Hodgkinson

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

96 papers	3,354 citations	32 h-index	53 g-index
113 ext. papers	3,670 ext. citations	4.2 avg, IF	5.57 L-index

#	Paper	IF	Citations
96	Characterization of crystalline and amorphous forms of irbesartan by multi-nuclear solid-state NMR.. *Solid State Nuclear Magnetic Resonance*, **2022**, 118, 101783	3.1	0
95	Paramagnetic solid-state NMR assignment and novel chemical conversion of the aldehyde group to dihydrogen ester and hemiacetal moieties in copper(ii)- and cobalt(ii)-pyridinecarboxaldehyde complexes.. *RSC Advances*, **2021**, 11, 20216-20231	3.7	2
94	Synthesis and structural characterization of cocrystals of isoniazid and cinnamic acid derivatives. *Journal of Molecular Structure*, **2020**, 1219, 128621	3.4	7
93	NMR crystallography of molecular organics. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2020**, 118-119, 10-53	10.4	49
92	Resolving alternative organic crystal structures using density functional theory and NMR chemical shifts. *Chemical Science*, **2020**, 11, 2987-2992	9.4	13
91	Towards Accurate Predictions of Proton NMR Spectroscopic Parameters in Molecular Solids. *ChemPhysChem*, **2020**, 21, 2075-2083	3.2	6
90	Improving Confidence in Crystal Structure Solutions Using NMR Crystallography: The Case of Piroxicam. *Crystal Growth and Design*, **2018**, 18, 3339-3351	3.5	20
89	Perspective: Current advances in solid-state NMR spectroscopy. *Journal of Chemical Physics*, **2018**, 149, 040901	3.9	21
88	Proton transfer in guanine-cytosine base pair analogues studied by NMR spectroscopy and PIMD simulations. *Faraday Discussions*, **2018**, 212, 331-344	3.6	17
87	Shape-selective crystallisation of fluxional carbon cages. *Chemical Science*, **2018**, 9, 8631-8636	9.4	15
86	Rationalising Heteronuclear Decoupling in Refocussing Applications of Solid-State NMR Spectroscopy. *ChemPhysChem*, **2017**, 18, 394-405	3.2	4
85	Structure and physicochemical characterization of a naproxen-picolinamide cocrystal. *Acta Crystallographica Section C, Structural Chemistry*, **2017**, 73, 168-175	0.8	20
84	Exploring Systematic Discrepancies in DFT Calculations of Chlorine Nuclear Quadrupole Couplings. *Journal of Physical Chemistry A*, **2017**, 121, 4103-4113	2.8	14
83	Perspectives: In crystallography we trust. *C&EN Global Enterprise*, **2016**, 94, 30-31	0.4	1
82	Stray-field NMR diffusion q-space diffraction imaging of monodisperse coarsening foams. *Journal of Colloid and Interface Science*, **2016**, 476, 20-28	9.3	1
81	Characterising the role of water in sildenafil citrate by NMR crystallography. *CrystEngComm*, **2016**, 18, 1054-1063	3.3	19
80	Temperature Dependence of NMR Parameters Calculated from Path Integral Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2016**, 12, 968-73	6.4	44

79	Characterization of Two Distinct Amorphous Forms of Valsartan by Solid-State NMR. *Molecular Pharmaceutics*, **2016**, 13, 211-22	5.6	25
78	Furosemide to one little hydrogen atom: NMR crystallography structure verification of powdered molecular organics. *Chemical Communications*, **2016**, 52, 6685-8	5.8	40
77	Visualization and processing of computed solid-state NMR parameters: MagresView and MagresPython. *Solid State Nuclear Magnetic Resonance*, **2016**, 78, 64-70	3.1	42
76	Testing the limits of NMR crystallography: the case of caffeine citric acid hydrate. *CrystEngComm*, **2016**, 18, 6700-6707	3.3	21
75	A furosemide isonicotinamide cocrystal: an investigation of properties and extensive structural disorder. *CrystEngComm*, **2015**, 17, 6707-6715	3.3	31
74	Na(+) mobility in sodium strontium silicate fast ion conductors. *Chemical Communications*, **2015**, 51, 1716-385	5.8	15
73	Resonance-assisted stabilisation of hydrogen bonds probed by NMR spectroscopy and path integral molecular dynamics. *Chemical Communications*, **2015**, 51, 13986-9	5.8	17
72	Simulating spin dynamics in organic solids under heteronuclear decoupling. *Solid State Nuclear Magnetic Resonance*, **2015**, 70, 28-37	3.1	5
71	Bisoprolol and bisoprolol-valsartan compatibility studied by differential scanning calorimetry, nuclear magnetic resonance and X-ray powder diffractometry. *Pharmaceutical Research*, **2015**, 32, 414-29	4.5	18
70	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	3.1	17
69	Solid-state NMR studies of nucleic acid components. *RSC Advances*, **2015**, 5, 12300-12310	3.7	21
68	Dynamics of water molecules and sodium ions in solid hydrates of nucleotides. *CrystEngComm*, **2014**, 16, 6756-6764	3.3	10
67	Effects of quantum nuclear delocalisation on NMR parameters from path integral molecular dynamics. *Chemistry - A European Journal*, **2014**, 20, 2201-7	4.8	47
66	A molecular dynamics study of the effects of fast molecular motions on solid-state NMR parameters. *CrystEngComm*, **2013**, 15, 8705	3.3	68
65	Well-tempered metadynamics as a tool for characterizing multi-component, crystalline molecular machines. *Journal of Physical Chemistry B*, **2013**, 117, 12286-95	3.4	14
64	NMR characterisation of dynamics in solvates and desolvates of formoterol fumarate. *Physical Chemistry Chemical Physics*, **2013**, 15, 6422-30	3.6	22
63	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	3.4	21
62	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, 176-86	3.9	21

61	Spectroscopic and structural characterization of the CyNHC adduct of B2pin2 in solution and in the solid state. *Journal of Organic Chemistry*, **2012**, 77, 785-9	4.2	111
60	NMR characterisation of structure in solvates and polymorphs of formoterol fumarate. *Magnetic Resonance in Chemistry*, **2012**, 50, 680-90	2.1	13
59	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	3.9	6
58	Solid-State NMR: Basic Principles & Practice **2012**,		108
57	Structural properties of carboxylic acid dimers confined within the urea tunnel structure: an MD simulation study. *Journal of Physical Chemistry B*, **2011**, 115, 2791-800	3.4	15
56	High-Resolution 1H NMR Spectroscopy of Solids. *Annual Reports on NMR Spectroscopy*, **2011**, 72, 185-223	1.7	37
55	Towards homonuclear J solid-state NMR correlation experiments for half-integer quadrupolar nuclei: experimental and simulated 11B MAS spin-echo dephasing and calculated 2J(BB) coupling constants for lithium diborate. *Physical Chemistry Chemical Physics*, **2011**, 13, 5778-89	3.6	31
54	Elucidation of structure and dynamics in solid octafluoronaphthalene from combined NMR, diffraction, and molecular dynamics studies. *Journal of the American Chemical Society*, **2010**, 132, 5179-85	16.4	22
53	Structures and phase transitions in (MoO2)2P2O7. *Inorganic Chemistry*, **2010**, 49, 2290-301	5.1	23
52	Computation and NMR crystallography of terbutaline sulfate. *Magnetic Resonance in Chemistry*, **2010**, 48 Suppl 1, S103-12	2.1	71
51	Understanding two-pulse phase-modulated decoupling in solid-state NMR. *Journal of Chemical Physics*, **2009**, 130, 114510	3.9	46
50	Use of rotary echoes in . *Chemical Physics Letters*, **2009**, 475, 58-63	2.5	12
49	Intramolecular Motion in Crystalline Organic Solids **2008**,		2
48	Structural characterisation of two pharmaceutically important steroids by solid-state NMR. *New Journal of Chemistry*, **2008**, 32, 1796	3.6	14
47	Characterization of Polymorphs and Solvates of Terbutaline Sulfate. *Crystal Growth and Design*, **2008**, 8, 80-90	3.5	34
46	Insights into homonuclear decoupling from efficient numerical simulation: techniques and examples. *Journal of Magnetic Resonance*, **2008**, 192, 183-96	3	23
45	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, 3416-23	3.6	57
44	On the orientational dependence of resolution in 1H solid-state NMR, and its role in MAS, CRAMPS and delayed-acquisition experiments. *Magnetic Resonance in Chemistry*, **2007**, 45 Suppl 1, S93-100	2.1	15

43	Using 17O solid-state NMR and first principles calculation to characterise structure and dynamics in inorganic framework materials. *Magnetic Resonance in Chemistry*, **2007**, 45 Suppl 1, S144-55	2.1	28
42	Chemical shift computations on a crystallographic basis: some reflections and comments. *Magnetic Resonance in Chemistry*, **2007**, 45 Suppl 1, S174-86	2.1	179
41	Structural study of polymorphs and solvates of finasteride. *Journal of Pharmaceutical Sciences*, **2007**, 96, 1380-97	3.9	57
40	Combining insights from solid-state NMR and first principles calculation: applications to the 19F NMR of octafluoronaphthalene. *Physical Chemistry Chemical Physics*, **2007**, 9, 2389-96	3.6	30
39	Quantification of homonuclear dipolar coupling networks from magic-angle spinning 1H NMR. *Molecular Physics*, **2006**, 104, 293-304	1.7	48
38	Origins of linewidth in 1H magic-angle spinning NMR. *Journal of Chemical Physics*, **2006**, 125, 144508	3.9	108
37	Quantitative analysis of 17O exchange and T1 relaxation data: application to zirconium tungstate. *Solid State Nuclear Magnetic Resonance*, **2006**, 30, 98-105	3.1	6
36	Characterization of oxygen dynamics in ZrW2O8. *Journal of the American Chemical Society*, **2005**, 127, 15175-81	16.4	29
35	Quantification of bambuterol hydrochloride in a formulated product using solid-state NMR. *Journal of Pharmaceutical and Biomedical Analysis*, **2005**, 38, 858-64	3.5	49
34	Heteronuclear decoupling in the NMR of solids. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2005**, 46, 197-222	10.4	96
33	Synthesis and NMR studies of 17O enriched AM2O8 phases. *Solid State Sciences*, **2005**, 7, 819-826	3.4	14
32	Characterisation of indomethacin and nifedipine using variable-temperature solid-state NMR. *Magnetic Resonance in Chemistry*, **2005**, 43, 881-92	2.1	56
31	Hydrogen bonding and dynamic behaviour in crystals and polymorphs of dicarboxylic-diamine adducts: a comparison between NMR parameters and X-ray diffraction studies. *Chemistry - A European Journal*, **2005**, 11, 7461-71	4.8	48
30	NMR studies of 31P, 1H spin pairs in solid tin(II) phosphite and tin(II) hydrogen phosphate. *Molecular Physics*, **2004**, 102, 877-882	1.7	5
29	Solid-state 109Ag CP/MAS NMR spectroscopy of some diammine silver(I) complexes. *Magnetic Resonance in Chemistry*, **2004**, 42, 819-26	2.1	20
28	Solid-state NMR studies of some tin(II) compounds. *Solid State Nuclear Magnetic Resonance*, **2004**, 26, 160-71	3.1	19
27	Resolution of 13C-19F interactions in the 13C NMR of spinning solids and liquid crystals. *Journal of Magnetic Resonance*, **2004**, 168, 124-31	3	8
26	The nature of oxygen exchange in ZrW2O8 revealed by two-dimensional solid-state 17O NMR. *Chemical Communications*, **2004**, 392-3	5.8	25

25	Heteronuclear decoupling in NMR of Liquid Crystals using continuous phase modulation. *Chemical Physics Letters*, **2003**, 368, 511-522	2.5	41
24	Improved heteronuclear decoupling schemes for solid-state magic angle spinning NMR by direct spectral optimization. *Chemical Physics Letters*, **2003**, 376, 259-267	2.5	60
23	Interference of homonuclear decoupling and exchange in the solid-state NMR of perfluorocyclohexane. *Journal of Magnetic Resonance*, **2003**, 161, 234-41	3	7
22	Transverse dephasing optimized solid-state NMR spectroscopy. *Journal of the American Chemical Society*, **2003**, 125, 13938-9	16.4	99
21	Improved Proton Decoupling in NMR Spectroscopy of Crystalline Solids Using the SPINAL-64 Sequence. *Monatshefte F Chemie*, **2002**, 133, 1549-1554	1.4	37
20	Improved Proton Decoupling in NMR Spectroscopy of Crystalline Solids Using the Spinal-64 Sequence **2002**, 69-74		1
19	Line-splitting and broadening effects from 19F in the 13CNMR of liquid crystals and solids. *Chemical Physics Letters*, **2001**, 344, 68-74	2.5	14
18	NMR studies of exchange between triazine rotamers *Magnetic Resonance in Chemistry*, **2000**, 38, 504-511	1.1	36
17	Simulation of extended periodic systems of nuclear spins. *Chemical Physics Letters*, **2000**, 326, 515-522	2.5	32
16	Numerical simulation of solid-state NMR experiments. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2000**, 36, 201-239	10.4	95
15	Homonuclear dipolar decoupling in solid-state NMR using continuous phase modulation. *Chemical Physics Letters*, **2000**, 319, 253-260	2.5	257
14	Experimental observation of periodic quasi-equilibria in solid-state NMR. *Chemical Physics Letters*, **1999**, 308, 381-389	2.5	28
13	The accuracy of distance measurements in solid-state NMR. *Journal of Magnetic Resonance*, **1999**, 139, 46-59	3	64
12	Quasi equilibria in solid-state NMR. *Chemical Physics Letters*, **1998**, 293, 110-118	2.5	18
11	Assignment and Measurement of Deuterium Quadrupolar Couplings in Liquid Crystals by Deuterium Carbon NMR Correlation Spectroscopy. *Journal of Physical Chemistry B*, **1998**, 102, 3718-3723	3.4	25
10	Deuterium to carbon cross-polarization in liquid crystals. *Journal of Chemical Physics*, **1998**, 109, 1873-1884	3.9	17
9	Sampling and the quantification of NMR data. *Advances in Magnetic and Optical Resonance*, **1997**, 20, 187-244		9
8	Cross-polarization efficiency in INS systems using adiabatic RF sweeps. *Journal of Chemical Physics*, **1997**, 107, 8742-8751	3.9	13

7	Deuterium–Carbon NMR Correlation Spectroscopy in Oriented Materials. *Journal of the American Chemical Society*, **1997**, 119, 12000-12001	16.4	18
6	The reliability of the determination of tensor parameters by solid-state nuclear magnetic resonance. *Journal of Chemical Physics*, **1997**, 107, 4808-4816	3.9	93
5	A Novel Detection–Estimation Scheme for Noisy NMR Signals: Applications to Delayed Acquisition Data. *Journal of Magnetic Resonance*, **1997**, 128, 30-41	3	89
4	Selective Data Acquisition in NMR. The Quantification of Anti-phase Scalar Couplings. *Journal of Magnetic Resonance Series A*, **1996**, 120, 18-30		11
3	Optimal Sampling Strategies for the Measurement of Spin–Spin Relaxation Times. *Journal of Magnetic Resonance Series B*, **1996**, 113, 25-34		88
2	Optimizing Spatially Localized NMR. *Journal of Magnetic Resonance Series B*, **1995**, 106, 261-269		5
1	Application of Maximum Entropy Methods to Three-Dimensional NMR Spectroscopy. *Journal of Magnetic Resonance Series B*, **1993**, 101, 218-222		10