Melinda J Duer

List of Publications by Year
in descending order

93 papers	3,715 citations	117453 34 h-index	138251 58 g-index
99 all docs	99 docs citations	99 times ranked	4922 citing authors

#	Article	IF	Citations
1	Dehydration and crystallization of amorphous calcium carbonate in solution and in air. Nature Communications, 2014, 5, 3169.	5.8	265
2	Citrate bridges between mineral platelets in bone. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E1354-63.	3.3	234
3	Tuning hardness in calcite by incorporation of amino acids. Nature Materials, 2016, 15, 903-910.	13.3	183
4	Site-Directed Surface Derivatization of MCM-41: Use of High-Resolution Transmission Electron Microscopy and Molecular Recognition for Determining the Position of Functionality within Mesoporous Materials. Angewandte Chemie - International Edition, 1998, 37, 2719-2723.	7.2	159
5	Structural information from quadrupolar nuclei in solid state NMR. Concepts in Magnetic Resonance Part A: Bridging Education and Research, 2006, 28A, 183-248.	0.2	136
6	The Organicâ'Mineral Interface in Bone Is Predominantly Polysaccharide. Chemistry of Materials, 2007, 19, 5055-5057.	3.2	132
7	The curious case of (caffeine)Â·(benzoic acid): how heteronuclear seeding allowed the formation of an elusive cocrystal. Chemical Science, 2013, 4, 4417.	3.7	115
8	The effect of particle agglomeration on the formation of a surface-connected compartment induced by hydroxyapatite nanoparticles inÂhuman monocyte-derived macrophages. Biomaterials, 2014, 35, 1074-1088.	5.7	114
9	Mineral Surface in Calcified Plaque Is Like That of Bone. Arteriosclerosis, Thrombosis, and Vascular Biology, 2008, 28, 2030-2034.	1.1	95
10	Investigation of the Nature of the Proteinâ'Mineral Interface in Bone by Solid-State NMR. Chemistry of Materials, 2005, 17, 3059-3061.	3.2	91
11	Enforcing Ostwald's rule of stages: Isolation of paracetamol forms III and II. European Journal of Pharmaceutical Sciences, 2007, 31, 271-276.	1.9	84
12	Applications of NMR Crystallography to Problems in Biomineralization: Refinement of the Crystal Structure and ³¹P Solid-State NMR Spectral Assignment of Octacalcium Phosphate. Journal of the American Chemical Society, 2012, 134, 12508-12515.	6.6	80
13	A model for a solvent-free synthetic organic research laboratory: click-mechanosynthesis and structural characterization of thioureas without bulk solvents. Green Chemistry, 2012, 14, 2462.	4.6	80
14	NMR Spectroscopy of Native and in Vitro Tissues Implicates PolyADP Ribose in Biomineralization. Science, 2014, 344, 742-746.	6.0	78
15	Probing the calcium and sodium local environment in bones and teeth using multinuclear solid state NMR and X-ray absorption spectroscopy. Physical Chemistry Chemical Physics, 2010, 12, 1081-1091.	1.3	70
16	The Mineral Phase of Calcified Cartilage: Its Molecular Structure and Interface with the Organic Matrix. Biophysical Journal, 2009, 96, 3372-3378.	0.2	67
17	The contribution of solid-state NMR spectroscopy to understanding biomineralization: Atomic and molecular structure of bone. Journal of Magnetic Resonance, 2015, 253, 98-110.	1.2	64
18	Collagen Structureâ€"Function Relationships from Solid-State NMR Spectroscopy. Accounts of Chemical Research, 2018, 51, 1621-1629.	7.6	63

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19	Carbide forming and cluster build-up reactions in ruthenium carbonyl cluster chemistry. Journal of Organometallic Chemistry, 1990, 383, 441-461.	0.8	59
20	Poly(ADP-Ribose) Links the DNA Damage Response and Biomineralization. Cell Reports, 2019, 27, 3124-3138.e13.	2.9	58
21	Glycation changes molecular organization and charge distribution in type I collagen fibrils. Scientific Reports, 2020, 10, 3397.	1.6	56
22	â€œPaddle-Wheelâ€•Tris(cyclopentadienyl)tin(II) and -lead(II) Complexes:Â Syntheses, Structures, and Model MO Calculations. Organometallics, 1997, 16, 3340-3351.	1.1	55
23	Solid-state NMR studies of the molecular motion in the kaolinite: DMSO intercalate. Journal of the American Chemical Society, 1992, 114, 6867-6874.	6.6	51
24	Potent New Heterogeneous Asymmetric Catalysts. Helvetica Chimica Acta, 2003, 86, 1753-1759.	1.0	50
25	Determination of structural data from multiple-quantum magic-angle spinning NMR experiments. Chemical Physics Letters, 1997, 277, 167-174.	1.2	46
26	A solid-state NMR study of the structure and molecular mobility of Î±-keratin. Physical Chemistry Chemical Physics, 2003, 5, 2894-2899.	1.3	43
27	2H NMR studies of single-component adsorption in silicalite: a comparative study of benzene and p-xylene. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 559.	1.7	40
28	Water brings order. Nature Materials, 2013, 12, 1081-1082.	13.3	40
29	Proline provides site-specific flexibility for in vivo collagen. Scientific Reports, 2018, 8, 13809.	1.6	40
30	Double-quantum-filtered nuclear magnetic resonance spectroscopy applied to quadrupolar nuclei in solids. Journal of Chemical Physics, 2002, 116, 710-722.	1.2	39
31	Probing the surface structure of hydroxyapatite using NMR spectroscopy and first principles calculations. Physical Chemistry Chemical Physics, 2008, 10, 600-606.	1.3	39
32	The Organicâ^'Mineral Interface in Teeth Is Like That in Bone and Dominated by Polysaccharides: Universal Mediators of Normal Calcium Phosphate Biomineralization in Vertebrates?. Chemistry of Materials, 2008, 20, 3549-3550.	3.2	38
33	Ligand fields from misdirected valency. 1. Lone-pair contributions in planar cobalt(II) Schiff-base complexes. Inorganic Chemistry, 1987, 26, 2573-2578.	1.9	36
34	The role of surface vanadia species in butane dehydrogenation over VOx/Al2O3. Catalysis Today, 2009, 142, 143-151.	2.2	35
35	Correlating quadrupolar nuclear spins: a multiple-quantum NMR approach. Chemical Physics Letters, 1999, 313, 763-770.	1.2	34
36	Pigmentation Chemistry and Radicalâ€Based Collagen Degradation in Alkaptonuria and Osteoarthritic Cartilage. Angewandte Chemie - International Edition, 2020, 59, 11937-11942.	7.2	34

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37	A solid-state NMR comparison of the mineral structure in bone from diseased joints in the horse. Journal of Materials Science, 2007, 42, 8804-8810.	1.7	33
38	Time-domain calculation of chemical exchange effects in the NMR spectra of rotating solids. Solid State Nuclear Magnetic Resonance, 1992, 1, 211-215.	1.5	32
39	Tannin Fingerprinting in Vegetable Tanned Leather by Solid State NMR Spectroscopy and Comparison with Leathers Tanned by Other Processes. Molecules, 2011, 16, 1240-1252.	1.7	32
40	Lipids in biocalcification: contrasts and similarities between intimal and medial vascular calcification and bone by NMR. Journal of Lipid Research, 2012, 53, 1569-1575.	2.0	30
41	Hydroxyproline Ring Pucker Causes Frustration of Helix Parameters in the Collagen Triple Helix. Scientific Reports, 2015, 5, 12556.	1.6	30
42	Ligand fields from misdirected valency. 2. Bent bonding in copper(II) acetylacetonates. Inorganic Chemistry, 1987, 26, 2578-2582.	1.9	28
43	An investigation of the structural units in sodium disilicate glass: a 2-D 29Si NMR study. Journal of Non-Crystalline Solids, 1995, 189, 107-117.	1.5	24
44	Chloroform encapsulated in p-tert-butylcalix[4]arene: Structure and dynamics. Physical Chemistry Chemical Physics, 2000, 2, 3977-3981.	1.3	24
45	Collagen atomic scale molecular disorder in ochronotic cartilage from an alkaptonuria patient, observed by solid state NMR. Journal of Inherited Metabolic Disease, 2011, 34, 1137-1140.	1.7	24
46	Bisphosphonate protonation states, conformations, and dynamics on bone mineral probed by solid-state NMR without isotope enrichment. European Journal of Pharmaceutics and Biopharmaceutics, 2010, 76, 120-126.	2.0	23
47	Evaluation of surface charge shift of collagen fibrils exposed to glutaraldehyde. Scientific Reports, 2018, 8, 10126.	1.6	23
48	Solid state 13C CP MAS NMR study of molecular motions and interactions of urea adsorbed on cotton cellulose. Physical Chemistry Chemical Physics, 2004, 6, 3175.	1.3	21
49	DNA Damage Response. Arteriosclerosis, Thrombosis, and Vascular Biology, 2020, 40, e193-e202.	1.1	21
50	Citrate Occurs Widely in Healthy and Pathological Apatitic Biomineral: Mineralized Articular Cartilage, and Intimal Atherosclerotic Plaque and Apatitic Kidney Stones. Calcified Tissue International, 2013, 93, 253-260.	1.5	20
51	NMR of Biopolymer-Apatite Composites: Developing a Model of the Molecular Structure of the Mineral-Matrix Interface in Calcium Phosphate Biomaterials. Chemistry of Materials, 2010, 22, 6109-6116.	3.2	19
52	Effect of Fluorination on Molecular Conformation in the Solid State: Tuning the Conformation of Cocrystal Formers. Crystal Growth and Design, 2011, 11, 972-981.	1.4	19
53	Bent bonds probed by ligand-field analysis. International Reviews in Physical Chemistry, 1990, 9, 227-280.	0.9	18
54	Solid state multinuclear NMR study of Ïƒ-acetylide complexes of platinum, trans-[ClPt(PnBu3)2î—¼Cî—¼Cî—¼pî—¼C6H4î—¸Cî—¼Cî—¼Pt(PnBu3)2Cl] and trans-[î—¸Pt(PnBu3)2î—¸Cî—¼Cî—¼pî—¼C6H4î—¸Cî— Magnetic Resonance, 1992, 1, 13-16.	1.5	16

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55	Contrasts between organic participation in apatite biomineralization in brachiopod shell and vertebrate bone identified by nuclear magnetic resonance spectroscopy. Journal of the Royal Society Interface, 2011, 8, 282-288.	1.5	16
56	Characterization of the phosphatic mineral of the barnacle Ibla cumingi at atomic level by solid-state nuclear magnetic resonance: comparison with other phosphatic biominerals. Journal of the Royal Society Interface, 2012, 9, 1510-1516.	1.5	16
57	Preparation of highly and generally enriched mammalian tissues for solid state NMR. Journal of Biomolecular NMR, 2015, 63, 119-123.	1.6	16
58	Tautomerism in 3{5}-(dimethoxyphenyl)pyrazoles. Acta Crystallographica Section B: Structural Science, 1996, 52, 746-752.	1.8	15
59	Solid-state13C and2H nuclear magnetic resonance studies of the benzeneâ€“hexafluorobenzene complex. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 823-826.	1.7	14
60	Applications of the CSA-amplified PASS experiment. Solid State Nuclear Magnetic Resonance, 2006, 30, 1-8.	1.5	14
61	Structural, Solid-State NMR and Theoretical Studies of the Inverse-Coordination of Lithium Chloride Using Group 13 Phosphide Hosts. Chemistry - A European Journal, 2007, 13, 1251-1260.	1.7	13
62	Essential but sparse collagen hydroxylysyl post-translational modifications detected by DNP NMR. Chemical Communications, 2018, 54, 12570-12573.	2.2	13
63	Solid state NMR - An indispensable tool in organic-inorganic biocomposite characterization; refining the structure of octacalcium phosphate composites with the linear metabolic di-acids succinate and adipate. Solid State Nuclear Magnetic Resonance, 2018, 95, 1-5.	1.5	13
64	Detection of nucleic acids and other low abundance components in native bone and osteosarcoma extracellular matrix by isotope enrichment and DNP-enhanced NMR. RSC Advances, 2019, 9, 26686-26690.	1.7	13
65	A cellular ligand-field model for â€˜l-lâ€™ spectral intensities. Molecular Physics, 1988, 64, 825-841.	0.8	12
66	A cellular ligand-field model for â€˜l-lâ€™ spectral intensities. Molecular Physics, 1988, 64, 793-823.	0.8	12
67	Decoupling residual dipolar coupling between 13C and14N spin pairs in CPMAS NMR. Solid State Nuclear Magnetic Resonance, 2006, 30, 130-134.	1.5	12
68	Incorporation of nanogels within calcite single crystals for the storage, protection and controlled release of active compounds. Chemical Science, 2021, 12, 9839-9850.	3.7	12
69	2H NMR studies of binary adsorption in silicalite. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 963.	1.7	11
70	A solid-state NMR investigation of the oddâ€“even effect in a series of liquid-crystal dimers. Physical Chemistry Chemical Physics, 2003, 5, 3034-3041.	1.3	11
71	Ligand fields from misdirected valency. 5. Consequences for spectral intensity distributions. Inorganic Chemistry, 1989, 28, 4260-4264.	1.9	9
72	Phospholipid headgroup dynamics in DOPG-d5-cytochrome c complexes as revealed by 2H and 31P NMR: The effects of a peripheral protein on collective lipid fluctuations. Solid State Nuclear Magnetic Resonance, 1997, 8, 55-64.	1.5	9

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73	Solid state NMR of salivary calculi: Proline-rich salivary proteins, citrate, polysaccharides, lipids, and organicâ€“mineral interactions. Comptes Rendus Chimie, 2016, 19, 1665-1671.	0.2	9
74	Mechanical adaptation of brachiopod shells via hydration-induced structural changes. Nature Communications, 2021, 12, 5383.	5.8	9
75	A cellular ligand-field model forl-lspectral intensities. Molecular Physics, 1993, 79, 1167-1194.	0.8	8
76	A cellular ligand-field model forl-lspectral intensities. Molecular Physics, 1993, 79, 1147-1165.	0.8	8
77	Molecular dynamics in crystalline C60Â·2CHBr3. Chemical Physics Letters, 2000, 321, 287-291.	1.2	8
78	A new glycation product â€˜norpronyl-lysine,â€™ and direct characterization of cross linking and other glycation adducts: NMR of model compounds and collagen. Bioscience Reports, 2014, 34, .	1.1	8
79	A ⁴³Ca nuclear magnetic resonance perspective on octacalcium phosphate and its hybrid derivatives. Magnetic Resonance in Chemistry, 2021, 59, 1048-1061.	1.1	8
80	Qualitative models for the NMR chemical shifts of interstitial atoms in clusters. Polyhedron, 1991, 10, 1749-1758.	1.0	7
81	Solid state NMR of isotope labelled murine fur: a powerful tool to study atomic level keratin structure and treatment effects. Journal of Biomolecular NMR, 2016, 66, 93-98.	1.6	7
82	Molecular conformations and dynamics in the extracellular matrix of mammalian structural tissues: Solid-state NMR spectroscopy approaches. Matrix Biology Plus, 2021, 12, 100086.	1.9	7
83	Ossicular density in golden moles (Chrysochloridae). Journal of Comparative Physiology A: Neuroethology, Sensory, Neural, and Behavioral Physiology, 2006, 192, 1349-1357.	0.7	6
84	The molecular glue binding organic matrix and mineral crystals in biominerals: Basic amino acids may be as important as acidic ones. Surface Science, 2010, 604, 1237-1238.	0.8	6
85	NMR studies of correlations between molecular motions and liquid-crystalline phase transitions in two hydrogen-bonded carboxylic acidâ€“pyridyl complexes. Part 2.â€”The alkyl regions. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 811-817.	1.7	5
86	29Si cross polarisation magic angle spinning spectroscopic studies on MCM-41 supported with metal carbonyl clusters. Inorganica Chimica Acta, 2003, 354, 75-78.	1.2	5
87	Rhodium(I) and palladium(II) complexes with the Schiff base 2,2â€²-bis((4S)-4-benzyl-2-oxazoline). Inorganica Chimica Acta, 2004, 357, 3351-3359.	1.2	5
88	NMR studies of correlations between molecular motions and liquid-crystalline phase transitions in two hydrogen-bonded carboxylic acidâ€“pyridyl complexes. Part 1.â€”The aromatic regions. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 803-810.	1.7	3
89	A Two-Dimensional NMR Experiment for the Study of Slow Motions in Complex Chemical Systems. Journal of Magnetic Resonance Series A, 1996, 119, 204-210.	1.6	2
90	Water desorption in Kelvin-probe force microscopy: a generic model. Nanotechnology, 2018, 29, 505705.	1.3	2

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91	225â€...The role of the dna damage response in vascular calcification. Heart, 2017, 103, A145.2-A146.	1.2	0
92	Pigmentierungschemie und radikalbasierter Kollagenabbau bei Alkaptonurie und Arthrose. Angewandte Chemie, 2020, 132, 12035-12040.	1.6	0
93	Innentitelbild: Pigmentierungschemie und radikalbasierter Kollagenabbau bei Alkaptonurie und Arthrose (Angew. Chem. 29/2020). Angewandte Chemie, 2020, 132, 11770-11770.	1.6	0