Melinda J Duer

List of Publications by Year in Descending Order

94 papers	3,016 citations	31 h-index	52 g-index
99 ext. papers	3,382 ext. citations	6.3 avg, IF	5.07 L-index

#	Paper	IF	Citations
94	Molecular conformations and dynamics in the extracellular matrix of mammalian structural tissues: Solid-state NMR spectroscopy approaches. *Matrix Biology Plus*, **2021**, 12, 100086	5.1	0
93	A Ca nuclear magnetic resonance perspective on octacalcium phosphate and its hybrid derivatives. *Magnetic Resonance in Chemistry*, **2021**, 59, 1048-1061	2.1	2
92	Mechanical adaptation of brachiopod shells via hydration-induced structural changes. *Nature Communications*, **2021**, 12, 5383	17.4	2
91	Incorporation of nanogels within calcite single crystals for the storage, protection and controlled release of active compounds. *Chemical Science*, **2021**, 12, 9839-9850	9.4	4
90	DNA Damage Response: A Molecular Lynchpin in the Pathobiology of Arteriosclerotic Calcification. *Arteriosclerosis, Thrombosis, and Vascular Biology*, **2020**, 40, e193-e202	9.4	10
89	Pigmentation Chemistry and Radical-Based Collagen Degradation in Alkaptonuria and Osteoarthritic Cartilage. *Angewandte Chemie - International Edition*, **2020**, 59, 11937-11942	16.4	20
88	Glycation changes molecular organization and charge distribution in type I collagen fibrils. *Scientific Reports*, **2020**, 10, 3397	4.9	17
87	Pigmentierungschemie und radikalbasierter Kollagenabbau bei Alkaptonurie und Arthrose. *Angewandte Chemie*, **2020**, 132, 12035-12040	3.6	
86	Innentitelbild: Pigmentierungschemie und radikalbasierter Kollagenabbau bei Alkaptonurie und Arthrose (Angew. Chem. 29/2020). *Angewandte Chemie*, **2020**, 132, 11770-11770	3.6	
85	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	3.7	9
84	Poly(ADP-Ribose) Links the DNA Damage Response and Biomineralization. *Cell Reports*, **2019**, 27, 3124-3138.e13	8.8	37
83	Collagen Structure-Function Relationships from Solid-State NMR Spectroscopy. *Accounts of Chemical Research*, **2018**, 51, 1621-1629	24.3	40
82	Evaluation of surface charge shift of collagen fibrils exposed to glutaraldehyde. *Scientific Reports*, **2018**, 8, 10126	4.9	15
81	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	3.1	8
80	Essential but sparse collagen hydroxylysyl post-translational modifications detected by DNP NMR. *Chemical Communications*, **2018**, 54, 12570-12573	5.8	11
79	Water desorption in Kelvin-probe force microscopy: a generic model. *Nanotechnology*, **2018**, 29, 505705	3.4	1
78	Proline provides site-specific flexibility for in vivo collagen. *Scientific Reports*, **2018**, 8, 13809	4.9	24

77	225 The role of the dna damage response in vascular calcification. *Heart*, **2017**, 103, A145.2-A146	5.1	
76	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	3	5
75	Solid state NMR of salivary calculi: Proline-rich salivary proteins, citrate, polysaccharides, lipids, and organic□mineral interactions. *Comptes Rendus Chimie*, **2016**, 19, 1665-1671	2.7	6
74	Tuning hardness in calcite by incorporation of amino acids. *Nature Materials*, **2016**, 15, 903-10	27	127
73	The contribution of solid-state NMR spectroscopy to understanding biomineralization: atomic and molecular structure of bone. *Journal of Magnetic Resonance*, **2015**, 253, 98-110	3	53
72	Preparation of highly and generally enriched mammalian tissues for solid state NMR. *Journal of Biomolecular NMR*, **2015**, 63, 119-23	3	14
71	Hydroxyproline Ring Pucker Causes Frustration of Helix Parameters in the Collagen Triple Helix. *Scientific Reports*, **2015**, 5, 12556	4.9	25
70	NMR spectroscopy of native and in vitro tissues implicates polyADP ribose in biomineralization. *Science*, **2014**, 344, 742-6	33.3	67
69	Dehydration and crystallization of amorphous calcium carbonate in solution and in air. *Nature Communications*, **2014**, 5, 3169	17.4	198
68	The effect of particle agglomeration on the formation of a surface-connected compartment induced by hydroxyapatite nanoparticles in human monocyte-derived macrophages. *Biomaterials*, **2014**, 35, 1074-88	15.6	98
67	A new glycation product 'norpronyl-lysine,' and direct characterization of cross linking and other glycation adducts: NMR of model compounds and collagen. *Bioscience Reports*, **2014**, 34,	4.1	8
66	Citrate bridges between mineral platelets in bone. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, E1354-63	11.5	195
65	The curious case of (caffeine)□(benzoic acid): how heteronuclear seeding allowed the formation of an elusive cocrystal. *Chemical Science*, **2013**, 4, 4417	9.4	97
64	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, 253-60	3.9	20
63	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, 12508-15	16.4	63
62	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	10	68
61	Lipids in biocalcification: contrasts and similarities between intimal and medial vascular calcification and bone by NMR. *Journal of Lipid Research*, **2012**, 53, 1569-75	6.3	26
60	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, 1510-6	4.1	15

59	Effect of Fluorination on Molecular Conformation in the Solid State: Tuning the Conformation of Cocrystal Formers. *Crystal Growth and Design*, **2011**, 11, 972-981	3.5	19
58	Collagen atomic scale molecular disorder in ochronotic cartilage from an alkaptonuria patient, observed by solid state NMR. *Journal of Inherited Metabolic Disease*, **2011**, 34, 1137-40	5.4	22
57	Mechanosynthesis of the Metallodrug Bismuth Subsalicylate from Bi2O3 and Structure of Bismuth Salicylate without Auxiliary Organic Ligands. *Angewandte Chemie*, **2011**, 123, 8004-8007	3.6	21
56	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, 282-8	4.1	13
55	Tannin fingerprinting in vegetable tanned leather by solid state NMR spectroscopy and comparison with leathers tanned by other processes. *Molecules*, **2011**, 16, 1240-52	4.8	25
54	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	9.6	19
53	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, 120-6	5.7	22
52	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, 1081-91	3.6	64
51	The molecular glue binding organic matrix and mineral crystals in biominerals: Basic amino acids may be as important as acidic ones: A perspective on the role of basic amino acids in the molecular recognition of hydroxyapatite by statherin using solid state NMR, by M. Ndao, J.T. Ash, P. Stayton, G. Drobny. *Surface Science*, **2010**, 604, 1237-1238	1.8	5
50	The role of surface vanadia species in butane dehydrogenation over VOx/Al2O3. *Catalysis Today*, **2009**, 142, 143-151	5.3	32
49	The mineral phase of calcified cartilage: its molecular structure and interface with the organic matrix. *Biophysical Journal*, **2009**, 96, 3372-8	2.9	58
48	Probing the surface structure of hydroxyapatite using NMR spectroscopy and first principles calculations. *Physical Chemistry Chemical Physics*, **2008**, 10, 600-6	3.6	36
47	The Organic–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	9.6	34
46	Mineral surface in calcified plaque is like that of bone: further evidence for regulated mineralization. *Arteriosclerosis, Thrombosis, and Vascular Biology*, **2008**, 28, 2030-4	9.4	86
45	The Organic–Mineral Interface in Bone Is Predominantly Polysaccharide. *Chemistry of Materials*, **2007**, 19, 5055-5057	9.6	117
44	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, 1251-60	4.8	13
43	Enforcing Ostwald's rule of stages: isolation of paracetamol forms III and II. *European Journal of Pharmaceutical Sciences*, **2007**, 31, 271-6	5.1	75
42	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	4.3	27

41	Applications of the CSA-amplified PASS experiment. *Solid State Nuclear Magnetic Resonance*, **2006**, 30, 1-8	3.1	13
40	Decoupling residual dipolar coupling between 13C and14N spin pairs in CPMAS NMR. *Solid State Nuclear Magnetic Resonance*, **2006**, 30, 130-4	3.1	11
39	Structural information from quadrupolar nuclei in solid state NMR. *Concepts in Magnetic Resonance Part A: Bridging Education and Research*, **2006**, 28A, 183-248	0.6	118
38	Ossicular density in golden moles (Chrysochloridae). *Journal of Comparative Physiology A: Neuroethology, Sensory, Neural, and Behavioral Physiology*, **2006**, 192, 1349-57	2.3	6
37	Investigation of the Nature of the Protein Mineral Interface in Bone by Solid-State NMR. *Chemistry of Materials*, **2005**, 17, 3059-3061	9.6	85
36	Inverse Coordination of an Ionic Lattice by a Metal Host. *Angewandte Chemie*, **2005**, 117, 5875-5879	3.6	6
35	Rhodium(I) and palladium(II) complexes with the Schiff base 2,2?-bis((4S)-4-benzyl-2-oxazoline). *Inorganica Chimica Acta*, **2004**, 357, 3351-3359	2.7	5
34	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	3.6	16
33	Potent New Heterogeneous Asymmetric Catalysts. *Helvetica Chimica Acta*, **2003**, 86, 1753-1759	2	44
32	29Si cross polarisation magic angle spinning spectroscopic studies on MCM-41 supported with metal carbonyl clusters. *Inorganica Chimica Acta*, **2003**, 354, 75-78	2.7	4
31	A solid-state NMR investigation of the odd Even effect in a series of liquid-crystal dimers. *Physical Chemistry Chemical Physics*, **2003**, 5, 3034-3041	3.6	10
30	A solid-state NMR study of the structure and molecular mobility of keratin. *Physical Chemistry Chemical Physics*, **2003**, 5, 2894-2899	3.6	36
29	Double-quantum-filtered nuclear magnetic resonance spectroscopy applied to quadrupolar nuclei in solids. *Journal of Chemical Physics*, **2002**, 116, 710-722	3.9	35
28	Molecular dynamics in crystalline C60 2CHBr3. *Chemical Physics Letters*, **2000**, 321, 287-291	2.5	7
27	Chloroform encapsulated in p-tert-butylcalix[4]arene: Structure and dynamics. *Physical Chemistry Chemical Physics*, **2000**, 2, 3977-3981	3.6	20
26	Correlating quadrupolar nuclear spins: a multiple-quantum NMR approach. *Chemical Physics Letters*, **1999**, 313, 763-770	2.5	30
25	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	16.4	134
24	Paddle-Wheel Tris(cyclopentadienyl)tin(II) and -lead(II) Complexes: Syntheses, Structures, and Model MO Calculations. *Organometallics*, **1997**, 16, 3340-3351	3.8	44

23	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	3.1	8
22	Determination of structural data from multiple-quantum magic-angle spinning NMR experiments. *Chemical Physics Letters*, **1997**, 277, 167-174	2.5	43
21	NMR studies of correlations between molecular motions and liquid-crystalline phase transitions in two hydrogen-bonded carboxylic acid–pyridyl complexes. Part 1.—The aromatic regions. *Journal of the Chemical Society, Faraday Transactions*, **1996**, 92, 803-810		3
20	NMR studies of correlations between molecular motions and liquid-crystalline phase transitions in two hydrogen-bonded carboxylic acid–pyridyl complexes. Part 2.—The alkyl regions. *Journal of the Chemical Society, Faraday Transactions*, **1996**, 92, 811-817		3
19	Tautomerism in 3{5}-(dimethoxyphenyl)pyrazoles. *Acta Crystallographica Section B: Structural Science*, **1996**, 52, 746-752		15
18	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		2
17	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	3.9	21
16	2 H 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		32
15	2 H NMR studies of binary adsorption in silicalite. *Journal of the Chemical Society, Faraday Transactions*, **1995**, 91, 963		8
14	Solid-state 13C and 2H nuclear magnetic resonance studies of the benzene–hexafluorobenzene complex. *Journal of the Chemical Society, Faraday Transactions*, **1993**, 89, 823-826		10
13	A cellular ligand-field model for l-l spectral intensities. *Molecular Physics*, **1993**, 79, 1167-1194	1.7	4
12	A cellular ligand-field model for l-l spectral intensities. *Molecular Physics*, **1993**, 79, 1147-1165	1.7	6
11	Solid-state NMR studies of the molecular motion in the kaolinite: DMSO intercalate. *Journal of the American Chemical Society*, **1992**, 114, 6867-6874	16.4	45
10	Time-domain calculation of chemical exchange effects in the NMR spectra of rotating solids. *Solid State Nuclear Magnetic Resonance*, **1992**, 1, 211-5	3.1	30
9	Solid state multinuclear NMR study of sigma-acetylide complexes of platinum, trans-[ClPt(PnBu3)2-C=C-p-C6H4-C=C-Pt(PnBu3)2Cl] and trans-[-Pt(PnBu3)2-C=C-p-C6H4-C=C-]n. *Solid State Nuclear Magnetic Resonance*, **1992**, 1, 13-6	3.1	15
8	Qualitative models for the NMR chemical shifts of interstitial atoms in clusters. *Polyhedron*, **1991**, 10, 1749-1758	2.7	4
7	Bent bonds probed by ligand-field analysis. *International Reviews in Physical Chemistry*, **1990**, 9, 227-280	7	16
6	Carbide forming and cluster build-up reactions in ruthenium carbonyl cluster chemistry. *Journal of Organometallic Chemistry*, **1990**, 383, 441-461	2.3	42

5	Ligand fields from misdirected valency. 5. Consequences for spectral intensity distributions. *Inorganic Chemistry*, **1989**, 28, 4260-4264	5.1	7
4	A cellular ligand-field model for [illegible] spectral intensities. *Molecular Physics*, **1988**, 64, 825-841	1.7	12
3	A cellular ligand-field model for [illegible] spectral intensities. *Molecular Physics*, **1988**, 64, 793-823	1.7	10
2	Ligand fields from misdirected valency. 2. Bent bonding in copper(II) acetylacetonates. *Inorganic Chemistry*, **1987**, 26, 2578-2582	5.1	20
1	Ligand fields from misdirected valency. 1. Lone-pair contributions in planar cobalt(II) Schiff-base complexes. *Inorganic Chemistry*, **1987**, 26, 2573-2578	5.1	30