

# Melinda J Duer

## List of Publications by Year in descending order

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93  
papers

3,715  
citations

117625

34  
h-index

138484

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. <i>Nature Communications</i> , 2014, 5, 3169.	12.8	265
2	Citrate bridges between mineral platelets in bone. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, E1354-63.	7.1	234
3	Tuning hardness in calcite by incorporation of amino acids. <i>Nature Materials</i> , 2016, 15, 903-910.	27.5	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. <i>Angewandte Chemie - International Edition</i> , 1998, 37, 2719-2723.	13.8	159
5	Structural information from quadrupolar nuclei in solid state NMR. <i>Concepts in Magnetic Resonance Part A: Bridging Education and Research</i> , 2006, 28A, 183-248.	0.5	136
6	The Organic-Mineral Interface in Bone Is Predominantly Polysaccharide. <i>Chemistry of Materials</i> , 2007, 19, 5055-5057.	6.7	132
7	The curious case of (caffeine)-(benzoic acid): how heteronuclear seeding allowed the formation of an elusive cocrystal. <i>Chemical Science</i> , 2013, 4, 4417.	7.4	115
8	The effect of particle agglomeration on the formation of a surface-connected compartment induced by hydroxyapatite nanoparticles in human monocyte-derived macrophages. <i>Biomaterials</i> , 2014, 35, 1074-1088.	11.4	114
9	Mineral Surface in Calcified Plaque Is Like That of Bone. <i>Arteriosclerosis, Thrombosis, and Vascular Biology</i> , 2008, 28, 2030-2034.	2.4	95
10	Investigation of the Nature of the Protein-Mineral Interface in Bone by Solid-State NMR. <i>Chemistry of Materials</i> , 2005, 17, 3059-3061.	6.7	91
11	Enforcing Ostwald's rule of stages: Isolation of paracetamol forms III and II. <i>European Journal of Pharmaceutical Sciences</i> , 2007, 31, 271-276.	4.0	84
12	Applications of NMR Crystallography to Problems in Biomineralization: Refinement of the Crystal Structure and $^{31}\text{P}$ Solid-State NMR Spectral Assignment of Octacalcium Phosphate. <i>Journal of the American Chemical Society</i> , 2012, 134, 12508-12515.	13.7	80
13	A model for a solvent-free synthetic organic research laboratory: click-mechanosynthesis and structural characterization of thioureas without bulk solvents. <i>Green Chemistry</i> , 2012, 14, 2462.	9.0	80
14	NMR Spectroscopy of Native and in Vitro Tissues Implicates PolyADP Ribose in Biomineralization. <i>Science</i> , 2014, 344, 742-746.	12.6	78
15	Probing the calcium and sodium local environment in bones and teeth using multinuclear solid state NMR and X-ray absorption spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1081-1091.	2.8	70
16	The Mineral Phase of Calcified Cartilage: Its Molecular Structure and Interface with the Organic Matrix. <i>Biophysical Journal</i> , 2009, 96, 3372-3378.	0.5	67
17	The contribution of solid-state NMR spectroscopy to understanding biomineralization: Atomic and molecular structure of bone. <i>Journal of Magnetic Resonance</i> , 2015, 253, 98-110.	2.1	64
18	Collagen Structure-Function Relationships from Solid-State NMR Spectroscopy. <i>Accounts of Chemical Research</i> , 2018, 51, 1621-1629.	15.6	63

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19	Carbide forming and cluster build-up reactions in ruthenium carbonyl cluster chemistry. <i>Journal of Organometallic Chemistry</i> , 1990, 383, 441-461.	1.8	59
20	Poly(ADP-Ribose) Links the DNA Damage Response and Biomineralization. <i>Cell Reports</i> , 2019, 27, 3124-3138.e13.	6.4	58
21	Glycation changes molecular organization and charge distribution in type I collagen fibrils. <i>Scientific Reports</i> , 2020, 10, 3397.	3.3	56
22	“Paddle-Wheel” Tris(cyclopentadienyl)tin(II) and -lead(II) Complexes: Syntheses, Structures, and Model MO Calculations. <i>Organometallics</i> , 1997, 16, 3340-3351.	2.3	55
23	Solid-state NMR studies of the molecular motion in the kaolinite: DMSO intercalate. <i>Journal of the American Chemical Society</i> , 1992, 114, 6867-6874.	13.7	51
24	Potent New Heterogeneous Asymmetric Catalysts. <i>Helvetica Chimica Acta</i> , 2003, 86, 1753-1759.	1.6	50
25	Determination of structural data from multiple-quantum magic-angle spinning NMR experiments. <i>Chemical Physics Letters</i> , 1997, 277, 167-174.	2.6	46
26	A solid-state NMR study of the structure and molecular mobility of $\alpha$ -keratin. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 2894-2899.	2.8	43
27	$^2\text{H}$ NMR studies of single-component adsorption in silicalite: a comparative study of benzene and p-xylene. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1995, 91, 559.	1.7	40
28	Water brings order. <i>Nature Materials</i> , 2013, 12, 1081-1082.	27.5	40
29	Proline provides site-specific flexibility for in vivo collagen. <i>Scientific Reports</i> , 2018, 8, 13809.	3.3	40
30	Double-quantum-filtered nuclear magnetic resonance spectroscopy applied to quadrupolar nuclei in solids. <i>Journal of Chemical Physics</i> , 2002, 116, 710-722.	3.0	39
31	Probing the surface structure of hydroxyapatite using NMR spectroscopy and first principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 600-606.	2.8	39
32	The Organic~Mineral Interface in Teeth Is Like That in Bone and Dominated by Polysaccharides: Universal Mediators of Normal Calcium Phosphate Biomineralization in Vertebrates?. <i>Chemistry of Materials</i> , 2008, 20, 3549-3550.	6.7	38
33	Ligand fields from misdirected valency. 1. Lone-pair contributions in planar cobalt(II) Schiff-base complexes. <i>Inorganic Chemistry</i> , 1987, 26, 2573-2578.	4.0	36
34	The role of surface vanadia species in butane dehydrogenation over $\text{VO}_x/\text{Al}_2\text{O}_3$ . <i>Catalysis Today</i> , 2009, 142, 143-151.	4.4	35
35	Correlating quadrupolar nuclear spins: a multiple-quantum NMR approach. <i>Chemical Physics Letters</i> , 1999, 313, 763-770.	2.6	34
36	Pigmentation Chemistry and Radical-Based Collagen Degradation in Alkaptonuria and Osteoarthritic Cartilage. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 11937-11942.	13.8	34

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37	A solid-state NMR comparison of the mineral structure in bone from diseased joints in the horse. <i>Journal of Materials Science</i> , 2007, 42, 8804-8810.	3.7	33
38	Time-domain calculation of chemical exchange effects in the NMR spectra of rotating solids. <i>Solid State Nuclear Magnetic Resonance</i> , 1992, 1, 211-215.	2.3	32
39	Tannin Fingerprinting in Vegetable Tanned Leather by Solid State NMR Spectroscopy and Comparison with Leathers Tanned by Other Processes. <i>Molecules</i> , 2011, 16, 1240-1252.	3.8	32
40	Lipids in biocalcification: contrasts and similarities between intimal and medial vascular calcification and bone by NMR. <i>Journal of Lipid Research</i> , 2012, 53, 1569-1575.	4.2	30
41	Hydroxyproline Ring Pucker Causes Frustration of Helix Parameters in the Collagen Triple Helix. <i>Scientific Reports</i> , 2015, 5, 12556.	3.3	30
42	Ligand fields from misdirected valency. 2. Bent bonding in copper(II) acetylacetonates. <i>Inorganic Chemistry</i> , 1987, 26, 2578-2582.	4.0	28
43	An investigation of the structural units in sodium disilicate glass: a 2-D <sup>29</sup> Si NMR study. <i>Journal of Non-Crystalline Solids</i> , 1995, 189, 107-117.	3.1	24
44	Chloroform encapsulated in p-tert-butylcalix[4]arene: Structure and dynamics. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 3977-3981.	2.8	24
45	Collagen atomic scale molecular disorder in ochronotic cartilage from an alkaptonuria patient, observed by solid state NMR. <i>Journal of Inherited Metabolic Disease</i> , 2011, 34, 1137-1140.	3.6	24
46	Bisphosphonate protonation states, conformations, and dynamics on bone mineral probed by solid-state NMR without isotope enrichment. <i>European Journal of Pharmaceutics and Biopharmaceutics</i> , 2010, 76, 120-126.	4.3	23
47	Evaluation of surface charge shift of collagen fibrils exposed to glutaraldehyde. <i>Scientific Reports</i> , 2018, 8, 10126.	3.3	23
48	Solid state <sup>13</sup> C CP MAS NMR study of molecular motions and interactions of urea adsorbed on cotton cellulose. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 3175.	2.8	21
49	DNA Damage Response. <i>Arteriosclerosis, Thrombosis, and Vascular Biology</i> , 2020, 40, e193-e202.	2.4	21
50	Citrate Occurs Widely in Healthy and Pathological Apatitic Biomineral: Mineralized Articular Cartilage, and Intimal Atherosclerotic Plaque and Apatitic Kidney Stones. <i>Calcified Tissue International</i> , 2013, 93, 253-260.	3.1	20
51	NMR of Biopolymer-Apatite Composites: Developing a Model of the Molecular Structure of the Mineral-Matrix Interface in Calcium Phosphate Biomaterials. <i>Chemistry of Materials</i> , 2010, 22, 6109-6116.	6.7	19
52	Effect of Fluorination on Molecular Conformation in the Solid State: Tuning the Conformation of Cocystal Formers. <i>Crystal Growth and Design</i> , 2011, 11, 972-981.	3.0	19
53	Bent bonds probed by ligand-field analysis. <i>International Reviews in Physical Chemistry</i> , 1990, 9, 227-280.	2.3	18
54	Solid state multinuclear NMR study of <i>trans</i> -[Pt(PnBu <sub>3</sub> ) <sub>2</sub> Cl] <sub>2</sub> and <i>trans</i> -[Pt(PnBu <sub>3</sub> ) <sub>2</sub> Cl] <sub>2</sub> . <i>Magnetic Resonance</i> , 1992, 1, 13-16.		

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55	Contrasts between organic participation in apatite biomineralization in brachiopod shell and vertebrate bone identified by nuclear magnetic resonance spectroscopy. <i>Journal of the Royal Society Interface</i> , 2011, 8, 282-288.	3.4	16
56	Characterization of the phosphatic mineral of the barnacle <i>Ibla cumingi</i> at atomic level by solid-state nuclear magnetic resonance: comparison with other phosphatic biominerals. <i>Journal of the Royal Society Interface</i> , 2012, 9, 1510-1516.	3.4	16
57	Preparation of highly and generally enriched mammalian tissues for solid state NMR. <i>Journal of Biomolecular NMR</i> , 2015, 63, 119-123.	2.8	16
58	Tautomerism in 3{5}-(dimethoxyphenyl)pyrazoles. <i>Acta Crystallographica Section B: Structural Science</i> , 1996, 52, 746-752.	1.8	15
59	Solid-state $^{13}\text{C}$ and $^2\text{H}$ nuclear magnetic resonance studies of the benzene-hexafluorobenzene complex. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1993, 89, 823-826.	1.7	14
60	Applications of the CSA-amplified PASS experiment. <i>Solid State Nuclear Magnetic Resonance</i> , 2006, 30, 1-8.	2.3	14
61	Structural, Solid-State NMR and Theoretical Studies of the Inverse-Coordination of Lithium Chloride Using Group 13 Phosphide Hosts. <i>Chemistry - A European Journal</i> , 2007, 13, 1251-1260.	3.3	13
62	Essential but sparse collagen hydroxylysyl post-translational modifications detected by DNP NMR. <i>Chemical Communications</i> , 2018, 54, 12570-12573.	4.1	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. <i>Solid State Nuclear Magnetic Resonance</i> , 2018, 95, 1-5.	2.3	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. <i>RSC Advances</i> , 2019, 9, 26686-26690.	3.6	13
65	A cellular ligand-field model for $^{1}\text{H}$ NMR spectral intensities. <i>Molecular Physics</i> , 1988, 64, 825-841.	1.7	12
66	A cellular ligand-field model for $^{1}\text{H}$ NMR spectral intensities. <i>Molecular Physics</i> , 1988, 64, 793-823.	1.7	12
67	Decoupling residual dipolar coupling between $^{13}\text{C}$ and $^{14}\text{N}$ spin pairs in CPMAS NMR. <i>Solid State Nuclear Magnetic Resonance</i> , 2006, 30, 130-134.	2.3	12
68	Incorporation of nanogels within calcite single crystals for the storage, protection and controlled release of active compounds. <i>Chemical Science</i> , 2021, 12, 9839-9850.	7.4	12
69	$^2\text{H}$ NMR studies of binary adsorption in silicalite. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1995, 91, 963.	1.7	11
70	A solid-state NMR investigation of the odd-even effect in a series of liquid-crystal dimers. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 3034-3041.	2.8	11
71	Ligand fields from misdirected valency. 5. Consequences for spectral intensity distributions. <i>Inorganic Chemistry</i> , 1989, 28, 4260-4264.	4.0	9
72	Phospholipid headgroup dynamics in DOPG-d5-cytochrome c complexes as revealed by $^2\text{H}$ and $^{31}\text{P}$ NMR: The effects of a peripheral protein on collective lipid fluctuations. <i>Solid State Nuclear Magnetic Resonance</i> , 1997, 8, 55-64.	2.3	9

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73	Solid state NMR of salivary calculi: Proline-rich salivary proteins, citrate, polysaccharides, lipids, and organicâ€“mineral interactions. <i>Comptes Rendus Chimie</i> , 2016, 19, 1665-1671.	0.5	9
74	Mechanical adaptation of brachiopod shells via hydration-induced structural changes. <i>Nature Communications</i> , 2021, 12, 5383.	12.8	9
75	A cellular ligand-field model for l-spectral intensities. <i>Molecular Physics</i> , 1993, 79, 1167-1194.	1.7	8
76	A cellular ligand-field model for l-spectral intensities. <i>Molecular Physics</i> , 1993, 79, 1147-1165.	1.7	8
77	Molecular dynamics in crystalline C60Âˆ2CHBr3. <i>Chemical Physics Letters</i> , 2000, 321, 287-291.	2.6	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. <i>Bioscience Reports</i> , 2014, 34, .	2.4	8
79	A <sup>43</sup> Ca nuclear magnetic resonance perspective on octacalcium phosphate and its hybrid derivatives. <i>Magnetic Resonance in Chemistry</i> , 2021, 59, 1048-1061.	1.9	8
80	Qualitative models for the NMR chemical shifts of interstitial atoms in clusters. <i>Polyhedron</i> , 1991, 10, 1749-1758.	2.2	7
81	Solid state NMR of isotope labelled murine fur: a powerful tool to study atomic level keratin structure and treatment effects. <i>Journal of Biomolecular NMR</i> , 2016, 66, 93-98.	2.8	7
82	Molecular conformations and dynamics in the extracellular matrix of mammalian structural tissues: Solid-state NMR spectroscopy approaches. <i>Matrix Biology Plus</i> , 2021, 12, 100086.	3.5	7
83	Ossicular density in golden moles ( <i>Chrysochloridae</i> ). <i>Journal of Comparative Physiology A: Neuroethology, Sensory, Neural, and Behavioral Physiology</i> , 2006, 192, 1349-1357.	1.6	6
84	The molecular glue binding organic matrix and mineral crystals in biominerals: Basic amino acids may be as important as acidic ones. <i>Surface Science</i> , 2010, 604, 1237-1238.	1.9	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. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1996, 92, 811-817.	1.7	5
86	<sup>29</sup> Si cross polarisation magic angle spinning spectroscopic studies on MCM-41 supported with metal carbonyl clusters. <i>Inorganica Chimica Acta</i> , 2003, 354, 75-78.	2.4	5
87	Rhodium(I) and palladium(II) complexes with the Schiff base 2,2â€“bis((4S)-4-benzyl-2-oxazoline). <i>Inorganica Chimica Acta</i> , 2004, 357, 3351-3359.	2.4	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. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1996, 92, 803-810.	1.7	3
89	A Two-Dimensional NMR Experiment for the Study of Slow Motions in Complex Chemical Systems. <i>Journal of Magnetic Resonance Series A</i> , 1996, 119, 204-210.	1.6	2
90	Water desorption in Kelvin-probe force microscopy: a generic model. <i>Nanotechnology</i> , 2018, 29, 505705.	2.6	2

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91	225â€¦The role of the dna damage response in vascular calcification. Heart, 2017, 103, A145.2-A146.	2.9	0
92	Pigmentierungschemie und radikalbasierter Kollagenabbau bei Alkaptonurie und Arthrose. Angewandte Chemie, 2020, 132, 12035-12040.	2.0	0
93	Innentitelbild: Pigmentierungschemie und radikalbasierter Kollagenabbau bei Alkaptonurie und Arthrose (Angew. Chem. 29/2020). Angewandte Chemie, 2020, 132, 11770-11770.	2.0	0