Ronald J Pugmire

List of Publications by Citations

131 papers	6,150 citations	44 h-index	75 g-index
141 ext. papers	6,529 ext. citations	6.3 avg, IF	4.9 L-index

#	Paper	IF	Citations
131	Carbon-13 solid-state NMR of Argonne-premium coals. *Energy & Fuels*, **1989**, 3, 187-193	4.1	470
130	Chemical model of coal devolatilization using percolation lattice statistics. *Energy & Fuels*, **1989**, 3, 175-186	4.1	347
129	Chemical percolation model for devolatilization. 3. Direct use of carbon-13 NMR data to predict effects of coal type. *Energy & Fuels*, **1992**, 6, 414-431	4.1	284
128	Cross polarization and magic angle sample spinning NMR spectra of model organic compounds. 3. Effect of the carbon-13-proton dipolar interaction on cross polarization and carbon-proton dephasing. *Journal of the American Chemical Society*, **1983**, 105, 6697-6704	16.4	224
127	Carbon-13 magnetic resonance. XXVI. A quantitative determination of the tautomeric populations of certain purines. *Journal of the American Chemical Society*, **1975**, 97, 4636-42	16.4	216
126	Chemical percolation model for devolatilization. 2. Temperature and heating rate effects on product yields. *Energy & Fuels*, **1990**, 4, 54-60	4.1	197
125	Cross polarization and magic angle sample spinning NMR spectra of model organic compounds. 1. Highly protonated molecules. *Journal of the American Chemical Society*, **1983**, 105, 2133-2141	16.4	162
124	Carbon-13 magnetic resonance. X. Six-membered nitrogen heterocycles and their cations. *Journal of the American Chemical Society*, **1968**, 90, 697-706	16.4	159
123	Carbon-13 magnetic resonance. XXV. A basic set of parameters for the investigation of tautomerism im purines. Established from carbon-13 magnetic resonance studies using certain purines and pyrrolo[2,3-d]pyrimidines. *Journal of the American Chemical Society*, **1975**, 97, 4627-36	16.4	156
122	Development and Application of a Correlation of 13C NMR Chemical Structural Analyses of Coal Based on Elemental Composition and Volatile Matter Content. *Energy & Fuels*, **1999**, 13, 60-68	4.1	140
121	A sensitive, high resolution magic angle turning experiment for measuring chemical shift tensor principal values. *Molecular Physics*, **1998**, 95, 1113-1126	1.7	126
120	Carbon-13 magnetic resonance. XIX. Benzimidazole, purine, and their anionic and cationic species. *Journal of the American Chemical Society*, **1971**, 93, 1880-1887	16.4	124
119	13C NMR Analysis of Soot Produced from Model Compounds and a Coal. *Energy & Fuels*, **2001**, 15, 961-971	4.1	120
118	Structural characterization of vitrinite-rich and inertinite-rich Permian-aged South African bituminous coals. *International Journal of Coal Geology*, **2008**, 76, 290-300	5.5	116
117	Cross polarization and magic angle sample spinning NMR spectra of model organic compounds. 2. Molecules of low or remote protonation. *Journal of the American Chemical Society*, **1983**, 105, 2142-2147	16.4	104
116	Carbon-13 magnetic resonance. XIV. Aza-analogs of polycyclic aromatic hydrocarbons. *Journal of the American Chemical Society*, **1969**, 91, 6381-6389	16.4	98
115	Production of Diethyl Carbonate from Ethanol and Carbon Monoxide over a Heterogeneous Catalyst. *Energy & Fuels*, **2002**, 16, 177-181	4.1	97

114	15N Chemical Shift Principal Values in Nitrogen Heterocycles. *Journal of the American Chemical Society*, **1997**, 119, 9804-9809	16.4	96
113	The Structure and Reaction Processes of Coal **1994**,		92
112	Carbon-13 magnetic resonance. XII. Five-membered nitrogen heterocycles and their charged species. *Journal of the American Chemical Society*, **1968**, 90, 4232-4238	16.4	89
111	15N Chemical Shift Tensors in Nucleic Acid Bases. *Journal of the American Chemical Society*, **1998**, 120, 9863-9869	16.4	76
110	Carbon-13 CP/MAS spectroscopy of coal macerals. *Fuel*, **1981**, 60, 717-722	7.1	76
109	Three-Dimensional Structure of the Siskin Green River Oil Shale Kerogen Model: A Comparison between Calculated and Observed Properties. *Energy & Fuels*, **2013**, 27, 702-710	4.1	75
108	Silica aerogel supported catalysts for Fischer Tropsch synthesis. *Applied Catalysis A: General*, **2005**, 278, 233-238	5.1	66
107	Nuclear magnetic resonance spectroscopy of soils and related materials. Relaxation of 13C nuclei in cross polarization nuclear magnetic resonance experiments. *Organic Geochemistry*, **1983**, 5, 121-129	3.1	66
106	Characterization of Macromolecular Structure Elements from a Green River Oil Shale, II. Characterization of Pyrolysis Products by 13C NMR, GC/MS, and FTIR. *Energy & Fuels*, **2014**, 28, 2959-2970	4.1	61
105	Characterization of fine particulate matter produced by combustion of residual fuel oil. *Journal of the Air and Waste Management Association*, **2000**, 50, 1106-14	2.4	61
104	Structural Determination in Carbonaceous Solids Using Advanced Solid State NMR Techniques. *Energy & Fuels*, **2001**, 15, 14-22	4.1	59
103	Effects of Hydrogen Bonding in the Calculation of 15N Chemical Shift Tensors: Benzamide. *Journal of the American Chemical Society*, **1996**, 118, 5488-5489	16.4	59
102	Revised structure of bistramide A (bistratene A): application of a new program for the automated analysis of 2D INADEQUATE spectra. *Journal of the American Chemical Society*, **1992**, 114, 1110-1111	16.4	57
101	Methyl Libration in Propane Measured with Neutron Inelastic Scattering. *Journal of Chemical Physics*, **1970**, 52, 4424-4436	3.9	55
100	Carbon-13 magnetic resonance. XX. 4-Azaindene (pyrrocoline) and related bridgehead nitrogen heterocycles. *Journal of the American Chemical Society*, **1971**, 93, 1887-1893	16.4	55
99	Carbon-13 magnetic resonance. XXII. The N-methylpurines. *Journal of the American Chemical Society* , **1973**, 95, 2791-6	16.4	55
98	Solid state magnetic resonance spectra of Illinois No. 6 coal and some reductive alkylation products. *Fuel*, **1984**, 63, 513-521	7.1	54
97	Carbon-13 magnetic resonance investigation of retinal isomers and related compounds. *Journal of the American Chemical Society*, **1974**, 96, 7008-14	16.4	54

96	Structural evolution of matched tar-char pairs in rapid pyrolysis experiments. *Fuel*, **1991**, 70, 414-423	7.1	50
95	Prediction of Sooting Tendency for Hydrocarbon Liquids in Diffusion Flames. *Energy & Fuels*, **2005**, 19, 2408-2415	4.1	49
94	Investigation of the Structural Conformation of Biphenyl by Solid State 13C NMR and Quantum Chemical NMR Shift Calculations. *Journal of Physical Chemistry A*, **2001**, 105, 6780-6784	2.8	48
93	Cross-polarization 13C-NMR spectroscopy with magic angle spinning characterizes organic matter in whole soils. *Nature*, **1981**, 294, 648-650	50.4	48
92	Production of diethyl carbonate from ethanol and carbon monoxide over a heterogeneous catalytic flow reactor. *Fuel Processing Technology*, **2003**, 83, 27-38	7.2	47
91	Characterization of Macromolecular Structure Elements from a Green River Oil Shale, I. Extracts. *Energy & Fuels*, **2014**, 28, 453-465	4.1	46
90	Carbon-13 magnetic resonance of coal-derived liquids. *Fuel*, **1977**, 56, 295-301	7.1	46
89	Measurement of 13C chemical shift tensor principal values with a magic-angle turning experiment. *Solid State Nuclear Magnetic Resonance*, **1994**, 3, 181-97	3.1	45
88	Solution and solid carbon-13 magnetic resonance study of the conformation of 9,10-dihydroanthracene and its 9,10-methylated derivatives. *Journal of the American Chemical Society*, **1981**, 103, 4817-4824	16.4	45
87	Technique for importing greater evolution resolution in multidimensional NMR spectrum. *Journal of Magnetic Resonance*, **1997**, 129, 134-44	3	44
86	Characterization of Macromolecular Structure of Pyrolysis Products from a Colorado Green River Oil Shale. *Industrial & Engineering Chemistry Research*, **2013**, 52, 15522-15532	3.9	43
85	15N CPMAS NMR of the Argonne Premium Coals. *Energy & Fuels*, **1997**, 11, 491-494	4.1	43
84	Carbon-13 Shift Tensors in Polycyclic Aromatic Compounds. 8.1 A Low-Temperature NMR Study of Coronene and Corannulene. *Journal of Physical Chemistry A*, **2000**, 104, 149-155	2.8	42
83	Improvements in the computerized analysis of 2D INADEQUATE spectra. *Analytical Chemistry*, **1992**, 64, 3133-49	7.8	38
82	A comparison of the carbon-13 n.m.r. spectra of solid coals and their liquids obtained by catalytic hydrogenation. *Fuel*, **1979**, 58, 11-16	7.1	38
81	Modeling Nitrogen Evolution during Coal Pyrolysis Based on a Global Free-Radical Mechanism. *Energy & Fuels*, **2000**, 14, 1094-1102	4.1	33
80	Solid State 15N and 13C NMR Study of Several Metal 5,10,15,20-Tetraphenylporphyrin Complexes. *Journal of the American Chemical Society*, **1997**, 119, 7114-7120	16.4	31
79	Chemical structure of char in the transition from devolatilization to combustion. *Energy & Fuels* , **1992**, 6, 643-650	4.1	31

78	A new high pressure sapphire nuclear magnetic resonance cell. *Review of Scientific Instruments*, **1996**, 67, 240-243	1.7	30
77	A simple synthesis of catalytically active, high surface area ceria aerogels. *Journal of Non-Crystalline Solids*, **2008**, 354, 5509-5514	3.9	28
76	Iron Aerogel and Xerogel Catalysts for Fischer□Tropsch Synthesis of Diesel Fuel. *Energy & Fuels* , **2009**, 23, 14-18	4.1	27
75	Quantitative determination of different carbon types in fusinite and anthracite coals from carbon-13 nuclear magnetic resonance chemical shielding line-shape analysis. *Analytical Chemistry*, **1988**, 60, 1574-1579	7.8	27
74	Carbon-13 NMR spectra of C-nucleosides. II. A study on the tautomerism of formycin and formycin B by the use of CMR spectroscopy. *Journal of Heterocyclic Chemistry*, **1973**, 10, 431-433	1.9	27
73	Rotational diffusion anisotropy in near ellipsoidal molecules. *Journal of the American Chemical Society*, **1973**, 95, 8465-8467	16.4	27
72	A New Method for Measuring the Graphite Content of Anthracite Coals and Soots. *Energy & Fuels*, **2002**, 16, 1296-1300	4.1	26
71	Modified spectral editing methods for (13)C CP/MAS experiments in solids. *Journal of Magnetic Resonance*, **2000**, 142, 326-30	3	26
70	Carbon-13 Chemical Shift Tensors and Molecular Conformation of Anisole. *The Journal of Physical Chemistry*, **1996**, 100, 8268-8272		25
69	Correlation of ring nitrogen substituents with carbon-13 nuclear magnetic resonance data in azoloazines. *Journal of Heterocyclic Chemistry*, **1987**, 24, 805-809	1.9	25
68	Torsional frequencies and barriers to methyl rotation in isobutylene, O -xylene, and durene. *Journal of Chemical Physics*, **1973**, 58, 1438-1445	3.9	25
67	Applications of the improved computerized analysis of 2D INADEQUATE spectra. *Analytical Chemistry*, **1992**, 64, 3150-60	7.8	24
66	Structural variations and evidence of segmental motion in the aliphatic region in coals observed with dipolar-dephasing NMR. *Energy & Fuels*, **1987**, 1, 50-55	4.1	24
65	Solid State NMR and Wide Angle X-ray Diffraction Studies of Supercritical Fluid CO2-Treated Poly(ethylene terephthalate). *Macromolecules*, **1998**, 31, 9238-9246	5.5	23
64	Carbon-13 NMR spectra of macerals separated from individual coals. *Organic Geochemistry*, **1982**, 4, 79-84	3.1	22
63	CO2 Clustering of 1-Decanol and Methanol in Supercritical Fluids by 13C Nuclear Spin□attice Relaxation. *Journal of Physical Chemistry B*, **1997**, 101, 2923-2928	3.4	21
62	Comparison of physical and chemical properties of maceral groups separated by density dradient centrifugation. *International Journal of Coal Geology*, **1985**, 5, 315-338	5.5	20
61	Solid-State NMR spectra and long, intra-dimer bonding in the pi-[TTF](2)(2+) (TTF = tetrathiafulvalene) dication. *Journal of Physical Chemistry A*, **2010**, 114, 6622-9	2.8	19

60	Silica Xerogel Supported Cobalt Metal Fischer‐Tropsch Catalysts for Syngas to Diesel Range Fuel Conversion. *Energy & Fuels*, **2004**, 18, 1519-1521	4.1	19
59	Carbon-13 nuclear relaxation measurements in nicotinamide adenine dinucleotide and adenosine monophosphate. *Journal of the American Chemical Society*, **1974**, 96, 2885-7	16.4	19
58	High resolution Chromatographic characterization of depolymerized coals of different rank: aliphatic and aromatic hydrocarbons. *Fuel*, **1992**, 71, 19-29	7.1	18
57	Cylindrical spinner and speed controller for magic angle spinning nuclear magnetic resonance. *Review of Scientific Instruments*, **1984**, 55, 516-520	1.7	18
56	The Effect of Coal Composition on Ignition and Flame Stability in Coaxial Oxy-Fuel Turbulent Diffusion Flames. *Energy & Fuels*, **2013**, 27, 4935-4945	4.1	17
55	Carbon-13 Chemical-Shift Tensors in Polycyclic Aromatic Compounds. 9.1 Biphenylene. *Journal of Physical Chemistry A*, **2000**, 104, 8290-8295	2.8	17
54	Carbon-13 chemical shift tensors in aromatic compounds. 4. Substituted naphthalenes. *Journal of the American Chemical Society*, **1992**, 114, 2832-2836	16.4	17
53	Application of new 13C n.m.r. techniques to the study of products from catalytic hydrodeoxygenation of SRC-II liquids. *Fuel*, **1984**, 63, 525-529	7.1	17
52	Modeling Light Gas and Tar Yields from Pyrolysis of Green River Oil Shale Demineralized Kerogen Using the Chemical Percolation Devolatilization Model. *Energy & Fuels*, **2015**, 29, 4921-4926	4.1	16
51	Study of the Evolution of Soot from Various Fuels. *Energy & Fuels*, **2005**, 19, 1804-1811	4.1	16
50	Dynamic nuclear polarization of nitrogen-15 in benzamide. *Solid State Nuclear Magnetic Resonance*, **1997**, 8, 129-37	3.1	15
49	Ring current effects in crystals. Evidence from 13C chemical shift tensors for intermolecular shielding in 4,7-di-t-butylacenaphthene versus 4,7-di-t-butylacenaphthylene. *Journal of Physical Chemistry A*, **2007**, 111, 2020-7	2.8	15
48	H and 15N Dynamic Nuclear Polarization Studies of Carbazole. *Journal of Physical Chemistry A*, **2000** , 104, 4413-4420	2.8	15
47	A study on the ring contraction of 5-diazo-1-methyluracil-6-methanolate and a convenient method for establishing the site of heterocyclic N-substitution. *Journal of Heterocyclic Chemistry*, **1974**, 11, 645-647	1.9	15
46	Carbon-13 NMR spectra of C-nucleosides. Showdomycin and Pseudouridine. *Journal of Heterocyclic Chemistry*, **1973**, 10, 427-429	1.9	15
45	Solid state NMR investigation of silica aerogel supported Fischer‐Tropsch catalysts. *Fuel Processing Technology*, **2007**, 88, 29-33	7.2	14
44	Structure determination of a new saponin from the plant Alphitonia zizyphoides by NMR spectroscopy. *Magnetic Resonance in Chemistry*, **1993**, 31, 472-480	2.1	14
43	The use of high-field carbon-13 NMR spectroscopy to characterize chiral centers in isopranes. *Magnetic Resonance in Chemistry*, **1986**, 24, 191-198	2.1	14

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41	Solid-state 13C NMR investigations of 4,7-dihydro-1H-tricyclopenta[def,jkl,pqr]triphenylene (sumanene) and indeno[1,2,3-cd]fluoranthene: Buckminsterfullerene moieties. *Physical Chemistry Chemical Physics*, **2010**, 12, 7934-41	3.6	13
40	Water Gas Shift Catalysis Using Iron Aerogels Doped with Palladium by the Gas-Phase Incorporation Method. *Energy & Fuels*, **2008**, 22, 1439-1443	4.1	13
39	The Study of Anthracene Aerosols by Solid-State NMR and ESR. *Energy & Fuels*, **2003**, 17, 738-743	4.1	13
38	Cluster Analysis of 13C Chemical Shift Tensor Principal Values in Polycyclic Aromatic Hydrocarbons. *Journal of Physical Chemistry A*, **2001**, 105, 7468-7472	2.8	13
37	A High-Resolution 3D Separated-Local-Field Experiment by Means of Magic-Angle Turning. *Journal of Magnetic Resonance*, **1997**, 126, 120-6	3	12
36	Solid-state NMR spectra and long intradimer bonds in the pi-[TCNE]22- dianion. *Journal of Physical Chemistry A*, **2006**, 110, 7962-9	2.8	12
35	Determination of 13C Chemical Shift Tensors in the Presence of Hydrogen Bonding and 14N Quadrupolar Coupling: p-Aminosalicylic Acid, Isoniazid, and Pyrazinamide. *Journal of Physical Chemistry A*, **2002**, 106, 11375-11379	2.8	12
34	15N Chemical Shift Tensors of HMX. *Journal of Physical Chemistry A*, **2002**, 106, 6352-6357	2.8	12
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32	Iron Ceria Aerogels Doped with Palladium as Water Gas Shift Catalysts for the Production of Hydrogen. *Industrial & Engineering Chemistry Research*, **2010**, 49, 1652-1657	3.9	10
31	Solid-State 13C NMR Measurements in Methoxynaphthalenes: Determination of the Substituent Chemical Shift Effects in the Principal Values. *Journal of Physical Chemistry A*, **1997**, 101, 9169-9175	2.8	10
30	15N NMR Chemical Shift Tensors of Substituted Hexaazaisowurtzitanes: The Intermediates in the Synthesis of CL-20 *Journal of Physical Chemistry A*, **2004**, 108, 2638-2644	2.8	10
29	Model Compound Study of the Pathways for Aromatic Hydrocarbon Formation in Soot. *Energy & Fuels*, **2007**, 21, 2584-2593	4.1	9
28	Carbon-13 Chemical-Shift Tensors in Polycyclic Aromatic Compounds: Fluoranthene and Decacyclene. *Journal of Physical Chemistry A*, **2002**, 106, 6477-6482	2.8	9
27	The Use of Anisotropic 13C Chemical Shifts To Study the Side-Chain Conformation of Polycrystalline 2-Methoxydibenzofuran. *Journal of the American Chemical Society*, **1995**, 117, 11984-11988	16.4	9
26	Fluid Structures of CO2 and CO2 CH4 Mixture at Supercritical Fluid and Liquid Densities by Nuclear Spin Lattice Relaxation Measurements. *Magnetic Resonance in Chemistry*, **1996**, 34, 479-488	2.1	9
25	New solid state NMR techniques in coal analysis. *TrAC - Trends in Analytical Chemistry*, **1984**, 3, 144-147	14.6	9

24	Carbon-13 NMR investigation of the protonation and quaternization of azoloazines with a bridgehead nitrogen. *Journal of Heterocyclic Chemistry*, **1976**, 13, 1057-1062	1.9	9
23	1H dynamic nuclear polarization in supercritical ethylene at 1.4 T. *Journal of Magnetic Resonance*, **2000**, 143, 233-9	3	8
22	13C NMR Techniques for Structural Studies of Coals and Coal Chars **1992**, 215-254		8
21	13C Chemical-shift tensors in an analogous series of heterosubstituted polycyclic aromatic compounds. *Magnetic Resonance in Chemistry*, **2001**, 39, 115-121	2.1	7
20	Improvements to the magic angle hopping experiment. *Solid State Nuclear Magnetic Resonance*, **1993**, 2, 235-43	3.1	7
19	Carbon-13 CP/MAS Study of Coal Macerals of Varying Rank. *ACS Symposium Series*, **1981**, 23-42	0.4	7
18	Carbon-13 NMR investigation of the structure of hydroxy-azoloazines with a bridgehead nitrogen. *Journal of Heterocyclic Chemistry*, **1977**, 14, 1403-1408	1.9	7
17	13C chemical shielding anisotropy studied by variable-angle sample spinning. *Journal of Magnetic Resonance*, **1987**, 71, 476-479		6
16	Solid-state 13C NMR investigations of cyclophanes: [2.2]paracyclophane and 1,8-dioxa[8](2,7)pyrenophane. *Journal of Physical Chemistry A*, **2012**, 116, 5193-8	2.8	5
15	A novel dipolar dephasing method for the slow magic angle turning experiment. *Journal of Magnetic Resonance*, **2001**, 152, 7-13	3	5
14	Use of relaxation agent doping to shorten very long spin-lattice relaxation times in a magic-angle turning experiment. *Solid State Nuclear Magnetic Resonance*, **1995**, 5, 257-62	3.1	5
13	Synthetic Doped Amorphous Ferrihydrite for the Fischer□Tropsch Synthesis of Alternative Fuels. *Industrial & Engineering Chemistry Research*, **2012**, 51, 4515-4522	3.9	4
12	Solid-state 13C NMR and quantum chemical investigation of metal diene complexes. *Magnetic Resonance in Chemistry*, **2007**, 45, 393-400	2.1	4
11	An efficient double-tuned 13C/1H probe circuit for CP/MAS NMR and its importance in linewidths. *Journal of Magnetic Resonance*, **1987**, 71, 485-494		4
10	Computerized analysis of 2D INADEQUATE spectra to assign chemical shifts in aromatic compounds. *Magnetic Resonance in Chemistry*, **1995**, 33, 803-811	2.1	3
9	Solid state structure of (pentamethylcyclopentadienyl)(2,4-dimethylpentadienyl)iron, Fe(C5Me5)(2,4-C7H11), and its incorporation into silica aerogels. *Polyhedron*, **2016**, 116, 76-81	2.7	2
8	A high-resolution (13)C 3D CSA-CSA-CSA correlation experiment by means of magic angle turning. *Journal of Magnetic Resonance*, **2000**, 145, 230-6	3	2
7	Modeling of the 15N and 13C Chemical Shift Tensors in Purine. *ACS Symposium Series*, **1999**, 162-176	0.4	2

6	Coal Structure from Solid State NMR **1996**,		2
5	Measurement of 13C Chemical-Shift Anisotropy in Coal. *Advances in Chemistry Series*, **1992**, 419-439		2
4	Glass and Crystal Formation in Binary Aromatic Mixtures: A Mechanism for Reducing Spin□lattice Relaxation Times. *The Journal of Physical Chemistry*, **1996**, 100, 18550-18553		1
3	Selective saturation and inversion of multiple resonances in high-resolution solid-state 13C experiments using slow spinning CP/MAS and tailored DANTE pulse sequences. *Solid State Nuclear Magnetic Resonance*, **1992**, 1, 185-95	3.1	1
2	Dynamic nuclear polarization of organic compound doped with free radicals. *Acta Physica Sinica (overseas Edition)*, **1998**, 7, 106-114		
1	An Integrated Spectroscopic Approach to the Chemical Characterization of Pyrolysis Oils. *ACS Symposium Series*, **1988**, 189-202	0.4	