Julio C Facelli

List of Publications by Year
in descending order

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193 papers	5,761 citations	125106 35 h-index	111975 67 g-index
220 all docs	220 docs citations	220 times ranked	5266 citing authors

#	Article	IF	Citations
1	Conformal Prediction in Clinical Medical Sciences. Journal of Healthcare Informatics Research, 2022, 6, 241-252.	5.3	5
2	K-means cluster analysis of cooperative effects of CO, NO2, O3, PM2.5, PM10, and SO2 on incidence of type 2 diabetes mellitus in the US. Environmental Research, 2022, 212, 113259.	3.7	4
3	Using supervised machine learning classifiers to estimate likelihood of participating in clinical trials of a de-identified version of ResearchMatch. Journal of Clinical and Translational Science, 2021, 5, e42.	0.3	8
4	A role for the MEGF6 gene in predisposition to osteoporosis. Annals of Human Genetics, 2021, 85, 58-72.	0.3	15
5	Human activity pattern implications for modeling SARS-CoV-2 transmission. Computer Methods and Programs in Biomedicine, 2021, 199, 105896.	2.6	15
6	Structure analysis of the proteins associated with polyA repeat expansion disorders. Journal of Biomolecular Structure and Dynamics, 2021, , 1-11.	2.0	1
7	Understanding protein structural changes for oncogenic missense variants. Heliyon, 2021, 7, e06013.	1.4	5
8	A Rare Variant in ERF (rs144812092) Predisposes to Prostate and Bladder Cancers in an Extended Pedigree. Cancers, 2021, 13, 2399.	1.7	4
9	An intronic variant in the CELF4 gene is associated with risk for colorectal cancer. Cancer Epidemiology, 2021, 72, 101941.	0.8	7
10	Data-driven identification of temporal glucose patterns in a large cohort of nondiabetic patients with COVID-19 using time-series clustering. JAMIA Open, 2021, 4, ooab063.	1.0	1
11	Microproteins: a 3D protein structure prediction analysis. Journal of Biomolecular Structure and Dynamics, 2021, , 1-9.	2.0	1
12	Alarm Settings of Continuous Glucose Monitoring Systems and Associations to Glucose Outcomes in Type 1 Diabetes. Journal of the Endocrine Society, 2020, 4, bvz005.	0.1	24
13	4549 Reproducible Informatics for Reproducible Translational Research. Journal of Clinical and Translational Science, 2020, 4, 66-67.	0.3	0
14	STHAM: an agent based model for simulating human exposure across high resolution spatiotemporal domains. Journal of Exposure Science and Environmental Epidemiology, 2020, 30, 459-468.	1.8	13
15	Associations Between the Time in Hypoglycemia and Hypoglycemia Awareness Status in Type 1 Diabetes Patients Using Continuous Glucose Monitoring Systems. Diabetes Technology and Therapeutics, 2020, 22, 787-793.	2.4	16
16	Temporal Pattern Detection to Predict Adverse Events in Critical Care: Case Study With Acute Kidney Injury. JMIR Medical Informatics, 2020, 8, e14272.	1.3	14
17	Generation and Classification of Activity Sequences for Spatiotemporal Modeling of Human Populations. Online Journal of Public Health Informatics, 2020, 12, e9.	0.4	7
18	Characterization of Analytic and Experimental Uncertainty of RNA-seq Co-expression Network Determination: Application to SCA2. , 2020, , .		0

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19	Magnesium interactions with a CX26 connexon in lipid bilayers. Journal of Molecular Modeling, 2019, 25, 232.	0.8	2
20	3048 Measuring the Autonomic Nervous System for Translational Research: Identification of Non-invasive Methods. Journal of Clinical and Translational Science, 2019, 3, 28-28.	0.3	1
21	The Effects of Calcium on Lipidâ€"Protein Interactions and Ion Flux in the Cx26 Connexon Embedded into a POPC Bilayer. Journal of Membrane Biology, 2019, 252, 451-464.	1.0	3
22	Study of the Lamellar and Micellar Phases of Pluronic F127: A Molecular Dynamics Approach. Processes, 2019, 7, 606.	1.3	3
23	Towards a content agnostic computable knowledge repository for data quality assessment. Computer Methods and Programs in Biomedicine, 2019, 177, 193-201.	2.6	17
24	Concept Bag: A New Method for Computing Concept Similarity in Biomedical Data. Lecture Notes in Computer Science, 2019, , 15-23.	1.0	0
25	A novel <scp>CDKN</scp>2A variant (p16^{L117P}) in a patient with familial and multiple primary melanomas. Pigment Cell and Melanoma Research, 2019, 32, 734-738.	1.5	7
26	An Architecture for Metadata-driven Integration of Heterogeneous Sensor and Health Data for Translational Exposomic Research. , 2019, , .		1
27	Looking Behind the Curtain: Identifying Factors Contributing to Changes on Care Outcomes During a Large Commercial EHR Implementation. EGEMS (Washington, DC), 2019, 7, 21.	2.0	10
28	An Architecture to Support Real-World Studies that Investigate the Autonomic Nervous System. Lecture Notes in Computer Science, 2019, , 196-203.	1.0	0
29	A Nonsynonymous Variant in the GOLM1 Gene in Cutaneous Malignant Melanoma. Journal of the National Cancer Institute, 2018, 110, 1380-1385.	3.0	23
30	Calcium interactions with Cx26 hemmichannel: Spatial association between MD simulations biding sites and variant pathogenicity. Computational Biology and Chemistry, 2018, 77, 331-342.	1.1	9
31	Comprehensive methodology to monitor longitudinal change patterns during EHR implementations: a case study at a large health care delivery network. Journal of Biomedical Informatics, 2018, 83, 40-53.	2.5	11
32	Mechanical properties of drug loaded diblock copolymer bilayers: A molecular dynamics study. Journal of Chemical Physics, 2018, 148, 214901.	1.2	6
33	Metadata Discovery of Heterogeneous Biomedical Datasets Using Token-Based Features. Lecture Notes in Electrical Engineering, 2018, , 60-67.	0.3	0
34	Generating Consistent Spatio-Temporal Events of Exposure for Translational Exposomic Research. ISEE Conference Abstracts, 2018, 2018, .	0.0	3
35	Effects of the enlargement of polyglutamine segments on the structure and folding of ataxin-2 and ataxin-3 proteins. Journal of Biomolecular Structure and Dynamics, 2017, 35, 504-519.	2.0	10
36	Gene co-expression network analysis for identifying modules and functionally enriched pathways in SCA2. Human Molecular Genetics, 2017, 26, 3069-3080.	1.4	40

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37	Development and classification of a robust inventory of near real-time outcome measurements for assessing information technology interventions in health care. Journal of Biomedical Informatics, 2017, 73, 62-75.	2.5	6
38	Diblock copolymer bilayers as model for polymersomes: A coarse grain approach. Journal of Chemical Physics, 2017, 146, 244904.	1.2	14
39	Molecular dynamics analysis of the aggregation propensity of polyglutamine segments. PLoS ONE, 2017, 12, e0178333.	1.1	22
40	Solving Interoperability in Translational Health. Applied Clinical Informatics, 2017, 08, 651-659.	0.8	1
41	Molecular dynamics simulations in drug delivery research: Calcium chelation of G3.5 PAMAM dendrimers. Cogent Chemistry, 2016, 2, 1229830.	2.5	12
42	A review of the applications of data mining and machine learning for the prediction of biomedical properties of nanoparticles. Computer Methods and Programs in Biomedicine, 2016, 132, 93-103.	2.6	89
43	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	0.5	445
44	Health information technology adoption: Understanding research protocols and outcome measurements for IT interventions in health care. Journal of Biomedical Informatics, 2016, 63, 33-44.	2.5	19
45	Predicting cytotoxicity of PAMAM dendrimers using molecular descriptors. Beilstein Journal of Nanotechnology, 2015, 6, 1886-1896.	1.5	20
46	Crystal structure prediction from first principles: The crystal structures of glycine. Chemical Physics Letters, 2015, 626, 20-24.	1.2	26
47	Development of an informatics infrastructure for data exchange of biomolecular simulations: Architecture, data models and ontology. SAR and QSAR in Environmental Research, 2015, 26, 577-593.	1.0	2
48	A domain analysis model for eIRB systems: Addressing the weak link in clinical research informatics. Journal of Biomedical Informatics, 2014, 52, 121-129.	2.5	8
49	Data model, dictionaries, and desiderata for biomolecular simulation data indexing and sharing. Journal of Cheminformatics, 2014, 6, 4.	2.8	11
50	The origin of the splitting of 13C and 15N NMR signals of 3(5)-phenyl-5(3)-methylpyrazolium chloride and bromide in the solid state: Quantum Espresso calculations. Journal of Molecular Structure, 2014, 1075, 551-558.	1.8	8
51	Development of a HIPAA-compliant environment for translational research data and analytics. Journal of the American Medical Informatics Association: JAMIA, 2014, 21, 185-189.	2.2	17
52	Structure prediction of polyglutamine disease proteins: comparison of methods. BMC Bioinformatics, 2014, 15, S11.	1.2	4
53	iBIOMES Lite: Summarizing Biomolecular Simulation Data in Limited Settings. Journal of Chemical Information and Modeling, 2014, 54, 1810-1819.	2.5	8
54	VIRGO: Virtual Identity Resolution on the Go. , 2014, , .		0

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55	Automatic Extraction of Nanoparticle Properties Using Natural Language Processing: NanoSifter an Application to Acquire PAMAM Dendrimer Properties. PLoS ONE, 2014, 9, e83932.	1.1	14
56	Structure and electronic properties of lithiumâ€“silicon clusters. Computational and Theoretical Chemistry, 2013, 1024, 61-68.	1.1	5
57	From NMR spectra to structure. Concepts in Magnetic Resonance Part A: Bridging Education and Research, 2013, 42, 261-289.	0.2	4
58	iBIOMES: Managing and Sharing Biomolecular Simulation Data in a Distributed Environment. Journal of Chemical Information and Modeling, 2013, 53, 726-736.	2.5	18
59	Optimization of Crystal Structures of Archetypical Pharmaceutical Compounds: A Plane-Wave DFT-D Study Using Quantum Espresso. Crystal Growth and Design, 2013, 13, 2181-2189.	1.4	28
60	Comparative pharmacokinetics of PAMAM-OH dendrimers and HPMA copolymers in ovarian tumor-bearing mice. Drug Delivery and Translational Research, 2013, 3, 260-271.	3.0	22
61	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.	2.5	94
62	A Service Oriented Framework to Assess the Quality of Electronic Health Data for Clinical Research. , 2013, , .		2
63	Implementing public health analytical services: Grid enabling of MetaMap. , 2013, , .		0
64	A Grid Based Approach to Share Public Health Surveillance Applications - The R Example. Online Journal of Public Health Informatics, 2013, 5, .	0.4	0
65	Utility of gene-specific algorithms for predicting pathogenicity of uncertain gene variants. Journal of the American Medical Informatics Association: JAMIA, 2012, 19, 207-211.	2.2	25
66	An agenda for ultra-large-scale system research for global health informatics. ACM SIGHIT Record, 2012, 2, 12-12.	0.5	2
67	Modeling of Asphaltenes: Assessment of Sensitivity of ¹³C Solid State NMR to Molecular Structure. Energy & Fuels, 2012, 26, 2161-2167.	2.5	15
68	Identification of pneumonia and influenza deaths using the death certificate pipeline. BMC Medical Informatics and Decision Making, 2012, 12, 37.	1.5	14
69	Consensus: a framework for evaluation of uncertain gene variants in laboratory test reporting. Genome Medicine, 2012, 4, 48.	3.6	10
70	Nanoinformatics: developing new computing applications for nanomedicine. Computing (Vienna/New) Tj ETQq0 0 0 rgBT /Overlock 10 T	3.2	15
71	Enabling GeneHunter as a Grid Service. Methods of Information in Medicine, 2011, 50, 364-371.	0.7	1
72	Characterization of uncertainty in the classification of multivariate assays: application to PAM50 centroid-based genomic predictors for breast cancer treatment plans. Journal of Clinical Bioinformatics, 2011, 1, 37.	1.2	20

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73	Towards crystal structure prediction of complex organic compounds â€“ a report on the fifth blind test. Acta Crystallographica Section B: Structural Science, 2011, 67, 535-551.	1.8	358
74	Chemical shift tensors: Theory and application to molecular structural problems. Progress in Nuclear Magnetic Resonance Spectroscopy, 2011, 58, 176-201.	3.9	106
75	Formation of one dimensional linear chains by Irâ€“Ir bonds in cis-dicarbonyldichloroiridate (I). Polyhedron, 2011, 30, 221-227.	1.0	6
76	Transition fromexotoendoCu absorption in CuSi_nclusters: a genetic algorithms density functional theory study. Molecular Simulation, 2011, 37, 678-688.	0.9	2
77	Understanding synchronization and hyper-synchronization in the the septo-hippocampal system. BMC Neuroscience, 2010, 11, .	0.8	0
78	Predicting the start week of respiratory syncytial virus outbreaks using real time weather variables. BMC Medical Informatics and Decision Making, 2010, 10, 68.	1.5	30
79	Septo-hippocampal networks in chronic epilepsy. Experimental Neurology, 2010, 222, 86-92.	2.0	20
80	Computational Feature Selection and Classification of RET Phenotypic Severity. Journal of Data Mining in Genomics & Proteomics, 2010, 01, .	0.5	5
81	SaTScan on a Cloud: On-Demand Large Scale Spatial Analysis of Epidemics. Online Journal of Public Health Informatics, 2010, 2, .	0.4	6
82	A case for using grid architecture for state public health informatics: the Utah perspective. BMC Medical Informatics and Decision Making, 2009, 9, 32.	1.5	8
83	Crystal structure prediction of flexible molecules using parallel genetic algorithms with a standard force field. Journal of Computational Chemistry, 2009, 30, 1973-1985.	1.5	29
84	Significant progress in predicting the crystal structures of small organic molecules â€“ a report on the fourth blind test. Acta Crystallographica Section B: Structural Science, 2009, 65, 107-125.	1.8	371
85	Intermolecular shielding contributions studied by modeling the C13 chemical-shift tensors of organic single crystals with plane waves. Journal of Chemical Physics, 2009, 131, 144503.	1.2	75
86	Parallel Genetic Algorithms for Crystal Structure Prediction: Successes and Failures in Predicting Bicalutamide Polymorphs. Lecture Notes in Computer Science, 2009, , 120-129.	1.0	0
87	Modeling NMR Chemical Shifts. , 2008, , 53-62.		10
88	A parallel genetic algorithm to discover patterns in genetic markers that indicate predisposition to multifactorial disease. Computers in Biology and Medicine, 2008, 38, 826-836.	3.9	9
89	Digital Sherpa. , 2008, , .		1
90	Molecular Structure and Carbon-13 Chemical Shielding Tensors Obtained from Nuclear Magnetic Resonance. Topics in Stereochemistry, 2007, , 1-61.	2.0	24

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91	A Distributed Computing Method for Crystal Structure Prediction of Flexible Molecules:â€‰ An Application to N-(2-Dimethyl-4,5-dinitrophenyl) Acetamide. Journal of Chemical Theory and Computation, 2007, 3, 201-209.	2.3	17
92	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, 2020-2027.	1.1	20
93	Solid-state13C NMR and quantum chemical investigation of metal diene complexes. Magnetic Resonance in Chemistry, 2007, 45, 393-400.	1.1	4
94	Modified genetic algorithms to model cluster structures in medium-sized silicon clusters:Si18â^'Si60. Physical Review A, 2006, 73, .	1.0	35
95	Computational Science and Engineering Online (CSE-Online):Â A Cyber-Infrastructure for Scientific Computing. Journal of Chemical Information and Modeling, 2006, 46, 971-984.	2.5	20
96	Design, Implementation and Deployment of a Commodity Cluster for Periodic Comparisons of Gene Sequences. , 2006, , 733-744.		0
97	Intermolecular shielding from molecular magnetic susceptibility. A new view of intermolecular ring current effects. Magnetic Resonance in Chemistry, 2006, 44, 401-408.	1.1	19
98	Modeling the13C chemical-shift tensor in organic single crystals by quantum mechanical methods: finite basis set effects. Magnetic Resonance in Chemistry, 2006, 44, 390-400.	1.1	22
99	Guest Editors' Foreword. Magnetic Resonance in Chemistry, 2006, 44, 195-196.	1.1	0
100	Poster reception---Digital Sherpa. , 2006, , .		0
101	A general framework to understand parallel performance in heterogeneous clusters: analysis of a new adaptive parallel genetic algorithm. Journal of Parallel and Distributed Computing, 2005, 65, 48-57.	2.7	26
102	Advances in Theoretical and Physical Aspects of Spinâ€"Spin Coupling Constants. ChemInform, 2005, 36, no.	0.1	0
103	A third blind test of crystal structure prediction. Acta Crystallographica Section B: Structural Science, 2005, 61, 511-527.	1.8	373
104	Global Optimization of Atomic Cluster Structures Using Parallel Genetic Algorithms. Materials Research Society Symposia Proceedings, 2005, 894, 1.	0.1	0
105	Theoretical study of the adsorption of H on Sin clusters, (n=3â€"10). Journal of Chemical Physics, 2005, 123, 214302.	1.2	24
106	Ab initioglobal optimization of the structures ofSinH,n=4â€"10, using parallel genetic algorithms. Physical Review A, 2005, 72, .	1.0	6
107	Modeling NMR Chemical Shift:â€‰ A Survey of Density Functional Theory Approaches for Calculating Tensor Properties. Journal of Physical Chemistry A, 2005, 109, 1180-1187.	1.1	67
108	Modified genetic algorithm to model crystal structures: III. Determination of crystal structures allowing simultaneous molecular geometry relaxation. International Journal of Quantum Chemistry, 2004, 96, 312-320.	1.0	17

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109	Calculations of chemical shieldings: Theory and applications. Concepts in Magnetic Resonance, 2004, 20A, 42-69.	1.3	94
110	Modeling solid-state effects on NMR chemical shifts using electrostatic models. Magnetic Resonance in Chemistry, 2004, 42, S41-S47.	1.1	19
111	Modified genetic algorithms to model atomic cluster structures: CuSi clusters. Computational and Theoretical Chemistry, 2004, 681, 149-155.	1.5	13
112	Modified genetic algorithms to model cluster structures in medium-size silicon clusters. Physical Review A, 2004, 69, .	1.0	54
113	Advances in Theoretical and Physical Aspects of Spinâ€“Spin Coupling Constants. Annual Reports on NMR Spectroscopy, 2003, 51, 167-260.	0.7	102
114	Indirect (J) coupling of inequivalent 75As nuclei in crystalline and glassy As2Se3 and As2S3. Journal of Chemical Physics, 2003, 119, 8519-8525.	1.2	7
115	Modified genetic algorithm to model crystal structures. II. Determination of a polymorphic structure of benzene using enthalpy minimization. Journal of Chemical Physics, 2002, 116, 5992-5995.	1.2	19
116	13C NMR Investigation of Solid-State Polymorphism in 10-Deacetyl Baccatin III. Journal of the American Chemical Society, 2002, 124, 10589-10595.	6.6	43
117	15N Chemical Shifts in Energetic Materials: CP/MAS and ab Initio Studies of Aminonitropyridines, Aminonitropyrimidines, and Their N-Oxides. International Journal of Molecular Sciences, 2002, 3, 858-872.	1.8	13
118	Modified genetic algorithm to model crystal structures. I. Benzene, naphthalene and anthracene. Journal of Chemical Physics, 2002, 116, 5984-5991.	1.2	69
119	Carbonates, Thiocarbonates, and the Corresponding Monoalkyl Derivatives: III. The 13C Chemical Shift Tensors in Potassium Carbonate, Bicarbonate and Related Monomethyl Derivatives. Solid State Nuclear Magnetic Resonance, 2002, 22, 29-49.	1.5	32
120	Cluster Analysis of 13C Chemical Shift Tensor Principal Values in Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2001, 105, 7468-7472.	1.1	16
121	13C Chemical-shift tensors in an analogous series of heterosubstituted polycyclic aromatic compounds. Magnetic Resonance in Chemistry, 2001, 39, 115-121.	1.1	7
122	Nitrogen-15 chemical shift in the pyridineâ€“methanol complex. Chemical Physics Letters, 2000, 322, 91-96.	1.2	15
123	Advances in theoretical and physical aspects of spin-spin coupling constants. Annual Reports on NMR Spectroscopy, 2000, 41, 55-184.	0.7	100
124	Carbon-13 Shift Tensors in Polycyclic Aromatic Compounds. 8.1A Low-Temperature NMR Study of Coronene and Corannulene. Journal of Physical Chemistry A, 2000, 104, 149-155.	1.1	47
125	Modeling of the 15N and 13C Chemical Shift Tensors in Purine. ACS Symposium Series, 1999, , 162-176.	0.5	3
126	A theoretical study of the acetate 13C chemical shift tensor in cadmium acetate dihydrate. Chemical Physics Letters, 1999, 302, 499-504.	1.2	22

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127	Effect of intramolecular interaction between polar and polarizable bonds on13C shielding constants in different conformations of 2-methoxy- and 2-vinyloxynaphthalene molecules: Anab initio study. Russian Chemical Bulletin, 1999, 48, 1054-1058.	0.4	1
128	Quantum mechanical calculations and experimental measurement of N-terminal charge effects on 1HN and 1HCÎ± chemical shifts in peptides. Biopolymers, 1998, 38, 573-581.	1.2	6
129	Modeling NMR chemical shifts: a comparison of charge models for solid state effects on 15N chemical shift tensors. Solid State Nuclear Magnetic Resonance, 1998, 10, 185-189.	1.5	36
130	Density Functional Theory Calculations of the Structure and the15N and13C Chemical Shifts of Methyl Bacteriopheophorbideaand Bacteriochlorophylla. Journal of Physical Chemistry B, 1998, 102, 2111-2116.	1.2	52
131	Carbon-13 Chemical Shift Tensors in Polycyclic Aromatic Compounds. 7.1 Symmetry Augmented Chemical Shiftâ^'Chemical Shift Correlation Spectroscopy and Single Crystal Study of Triphenylene. Journal of the American Chemical Society, 1998, 120, 9305-9311.	6.6	30
132	15N Chemical Shift Tensors in Nucleic Acid Bases. Journal of the American Chemical Society, 1998, 120, 9863-9869.	6.6	80
133	NMR at Cryogenic Temperatures:Â A13C NMR Study of Ferrocene. Journal of Physical Chemistry A, 1998, 102, 7692-7697.	1.1	21
134	Nitrogen-15 Chemical Shifts in AT (Adenine-Thymine) and CG (Cytosine-Guanine) Nucleic Acid Base Pairs. Journal of Biomolecular Structure and Dynamics, 1998, 16, 619-629.	2.0	7
135	15N Chemical Shift Principal Values in Nitrogen Heterocycles. Journal of the American Chemical Society, 1997, 119, 9804-9809.	6.6	106
136	Solid State15N and13C NMR Study of Several Metal 5,10,15,20-Tetraphenylporphyrin Complexes. Journal of the American Chemical Society, 1997, 119, 7114-7120.	6.6	34
137	Solid-State 13C NMR Measurements in Methoxynaphthalenes:â€‰ Determination of the Substituent Chemical Shift Effects in the Principal Values. Journal of Physical Chemistry A, 1997, 101, 9169-9175.	1.1	11
138	Experimental and Theoretical Study of the Ethoxy Group Conformational Effect on13C Chemical Shifts inOrtho-Substituted Phenetols. Magnetic Resonance in Chemistry, 1997, 35, 351-356.	1.1	15
139	Effects of Hydrogen Bonding in the Calculation of15N Chemical Shift Tensors:Â Benzamide. Journal of the American Chemical Society, 1996, 118, 5488-5489.	6.6	63
140	13C Dipolar NMR Spectrum of Matrix-Isolated o-Benzyne-1,2-13C2. Journal of the American Chemical Society, 1996, 118, 846-852.	6.6	72
141	Carbon-13 Chemical Shift Tensors in Polycyclic Aromatic Compounds. 6.1Single-Crystal Study of Perylene. Journal of the American Chemical Society, 1996, 118, 4880-4888.	6.6	42
142	Carbon-13 Chemical Shift Tensors and Molecular Conformation of Anisole. The Journal of Physical Chemistry, 1996, 100, 8268-8272.	2.9	28
143	Relationship of 13C NMR chemical shift tensors to diffraction structures. Acta Crystallographica Section B: Structural Science, 1995, 51, 540-546.	1.8	43
144	Carbon-13 chemical shift tensors of carboxylic acids: GIAO calculations in acetic acid + methylamine dimer. Molecular Physics, 1995, 86, 865-872.	0.8	37

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145	15N Chemical Shift Tensors of Uracil Determined from 15N Powder Pattern and 15N-13C Dipolar NMR Spectroscopy. The Journal of Physical Chemistry, 1995, 99, 10454-10458.	2.9	38
146	Low-Temperature 13C Magnetic Resonance. 9.Steric Effects for Methyl Chemical Shift Tensors in Methylcyclohexanes. Journal of the American Chemical Society, 1995, 117, 8441-8446.	6.6	18
147	Carbon-13 Chemical Shift Tensors in Polycyclic Aromatic Compounds. 5. Single-Crystal Study of Acenaphthene. Journal of the American Chemical Society, 1995, 117, 2336-2343.	6.6	56
148	Solid-State 13C NMR, X-ray, and Quantum Mechanical Studies of the Carbon Chemical Shifts Tensors of p-Tolyl Ether. The Journal of Physical Chemistry, 1994, 98, 12186-12190.	2.9	13
149	Ab initio study of the internal rotation barrier of formamide and the formamide-H2O complex. International Journal of Quantum Chemistry, 1993, 45, 123-132.	1.0	30
150	Determination of molecular symmetry in crystalline naphthalene using solid-state NMR. Nature, 1993, 365, 325-327.	13.7	109
151	Proximity effects on the nuclear magnetic shielding tensor. Computational and Theoretical Chemistry, 1993, 281, 61-66.	1.5	8
152	Effects of electronic resonance interaction on methoxy group NMR parameters: theoretical and experimental study of substituted 2-methoxypyridines. The Journal of Physical Chemistry, 1993, 97, 91-93.	2.9	23
153	Carbon-13 Chemical Shielding Tensors in Sugars: Sucrose and Methyl-Î±-D-Glucopyranoside. , 1993, , 367-384.		26
154	Ab initio and oxygen-17 NMR studies of the substituent effects on the tautomeric equilibrium in 6-X-(1H)-2-pyridones. The Journal of Physical Chemistry, 1992, 96, 7895-7898.	2.9	19
155	Effects of protonation on acetone: nuclear magnetic resonance and ab initio studies. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 2459-2463.	1.7	36
156	Carbon-13 chemical shift tensors in aromatic compounds. 4. Substituted naphthalenes. Journal of the American Chemical Society, 1992, 114, 2832-2836.	6.6	21
157	Carbon-13 chemical shift tensors in aromatic compounds. 3. Phenanthrene and triphenylene. Journal of the American Chemical Society, 1992, 114, 2826-2832.	6.6	16
158	Nonplanarity of the methoxy groups in o-dimethoxybenzene: quantum chemical calculations of the 17O chemical shieldings. Computational and Theoretical Chemistry, 1992, 276, 307-313.	1.5	7
159	Carbon-13 chemical shift tensors in polycyclic aromatic compounds. 2. Single-crystal study of naphthalene. Journal of the American Chemical Society, 1991, 113, 750-753.	6.6	59
160	Ab initio study of cyclobutadiene and its aza-substituted derivatives. Ground state properties and vibrational frequencies. Computational and Theoretical Chemistry, 1991, 236, 119-133.	1.5	9
161	COMPARISON OF 13C CHEMICAL SHIELDING ANISOTROPY IN MODEL COMPOUNDS & COALS WITH THEORETICAL VALUES. , 1991, , 72-75.		0
162	New theoretical results on the COâ€¦cyclobutadiene complex. Chemical Physics Letters, 1990, 173, 21-25.	1.2	3

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163	A comparison of the IGLO and LORG methods for the calculations of nuclear magnetic shieldings. Journal of Computational Chemistry, 1990, 11, 32-44.	1.5	47
164	Ab initio and oxygen-17 NMR study of aromatic compounds with dicoordinate oxygen atoms. 1. Methoxy- and (methylenedioxy)benzene derivatives. The Journal of Physical Chemistry, 1990, 94, 7418-7423.	2.9	19
165	Experimental and theoretical study of the methoxy group conformational effect on13C chemical shifts inortho-substituted anisoles. Magnetic Resonance in Chemistry, 1989, 27, 158-161.	1.1	42
166	Ab initio molecular orbital studies of chemical shielding in transition-metal compounds: molybdenum-95 shielding in molybdate and thiomolybdate [MoOnS(4-n)]2- anions. Journal of the American Chemical Society, 1989, 111, 7619-7621.	6.6	20
167	Low-temperature carbon-13 magnetic resonance. 8. Chemical shielding anisotropy of olefinic carbons. Journal of the American Chemical Society, 1988, 110, 3386-3392.	6.6	33
168	Carbon-13 NMR and polarized IR spectra of vicinally labeled cyclobutadiene-13C2 in an argon matrix: interconversion of valence tautomers. Journal of the American Chemical Society, 1988, 110, 2648-2650.	6.6	77
169	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.	3.2	29
170	Carbon-13 chemical-shift tensors in single-crystal methoxybenzenes. Journal of the Chemical Society Faraday Transactions I, 1988, 84, 3673.	1.0	42
171	The effect of transverse cross relaxation on nuclear magnetic resonance dipolar spectra. Journal of Chemical Physics, 1988, 89, 5542-5546.	1.2	8
172	13C Dipolar spectroscopy of nitromethane. Molecular Physics, 1988, 64, 1031-1040.	0.8	8
173	Carbon-13 shielding tensors: experimental and theoretical determination. Accounts of Chemical Research, 1987, 20, 152-158.	7.6	45
174	Carbon-13 chemical shielding tensors in polycyclic aromatic compounds. 1. Single-crystal study of pyrene. Journal of the American Chemical Society, 1987, 109, 2639-2644.	6.6	34
175	Theoretical study of the in-plane components of the 13C shielding tensors in condensed aromatic hydrocarbons. Theoretica Chimica Acta, 1987, 71, 277-288.	0.9	27
176	Analysis of the IGLO bond contributions to the13C shielding tensors in the local bond frame. International Journal of Quantum Chemistry, 1987, 31, 45-55.	1.0	11
177	Low-temperature carbon-13 magnetic resonance in solids. 7. Methyl carbons. Journal of the American Chemical Society, 1986, 108, 6464-6470.	6.6	34
178	Low-temperature carbon-13 magnetic resonance in solids. 6. Methine carbons. Journal of the American Chemical Society, 1986, 108, 4268-4272.	6.6	27
179	Low temperature 13C NMR magnetic resonance in solids 4. Cyclopropane, bicyclo[1.1.0]butane and [1.1.1] propellane. Theoretica Chimica Acta, 1985, 68, 421-430.	0.9	36
180	Low-temperature carbon-13 magnetic resonance in solids. 5. Chemical shielding anisotropy of the 13CH2 group. Journal of the American Chemical Society, 1985, 107, 6749-6754.	6.6	38

#	Article	IF	Citations
181	Iglo calculations of the antisymmetric components of nuclear magnetic shielding tensors. Chemical Physics Letters, 1984, 112, 147-149.	1.2	27
182	A long-lived molecular association between acetone and 2-methoxy-5-aminopyridine. Magnetic Resonance in Chemistry, 1984, 22, 245-249.	0.7	1
183	A theoretical study of medium effects on the transmission mechanisms of the fermi contact term of spin-spin coupling constants in the acetamide molecule. International Journal of Quantum Chemistry, 1984, 25, 515-525.	1.0	2
184	Low-temperature carbon-13 magnetic resonance in solids. 3. Linear and pseudolinear molecules. Journal of the American Chemical Society, 1984, 106, 7672-7676.	6.6	143
185	Importance of multicenter integrals in semiempirical calculations of nuclear spin-spin coupling constants. 1. Isotropic coupling. Journal of the American Chemical Society, 1984, 106, 3407-3413.	6.6	12
186	Nuclear magnetic resonance and PCILO study of the side-chain conformations in m-anisaldehyde and 2,5-dimethoxybenzaldehyde. The Journal of Physical Chemistry, 1983, 87, 2603-2607.	2.9	15
187	The use of partially restricted molecular orbitals to investigate transmission mechanisms of spin-spin coupling constants. IIIâ€"an INDO study of long-range Fï£¿H couplings in fluorinated derivatives of toluene. Magnetic Resonance in Chemistry, 1982, 19, 138-143.	0.7	19
188	A proton NMR analysis of the OCH3 group conformation in 2-methoxypyridines. Magnetic Resonance in Chemistry, 1982, 20, 40-41.	0.7	19
189	Transmission mechanisms of inter-proton long-range couplings in substituted anisoles. Magnetic Resonance in Chemistry, 1981, 17, 199-203.	0.7	32
190	The use of partially restricted molecular orbitals to investigate transmission mechanisms of spin-spin coupling constants. I. The? and? contributions within the FPT INDO method. Theoretica Chimica Acta, 1981, 59, 17-24.	0.9	43
191	Inclusion of hydrogenp orbitals in the semiempirical calculation ofNMR parameters. III:INDO CHF calculations of orbital and dipolar contributions to spin-spin coupling constants involving protons. International Journal of Quantum Chemistry, 1981, 20, 909-919.	1.0	8
192	Influence of the INDO parameterization on the indirect spin-spin coupling constants as calculated by the FPT INDO method. Magnetic Resonance in Chemistry, 1980, 13, 137-142.	0.7	14
193	Population Analysis with Hydrogen 2 p Polarization Functions Included in the INDO Basis Set. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1980, 35, 1350-1353.	0.7	0