

Cynthia J Jameson

List of Publications by Year in descending order

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81900

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200
docs citations

200
times ranked

2505
citing authors

#	ARTICLE	IF	CITATIONS
1	Gas-phase ¹³ C chemical shifts in the zero-pressure limit: refinements to the absolute shielding scale for ¹³ C. Chemical Physics Letters, 1987, 134, 461-466.	2.6	398
2	Density Dependence of ¹²⁹ Xe Chemical Shifts in Mixtures of Xenon and Other Gases. Journal of Chemical Physics, 1970, 53, 2310-2321.	3.0	189
3	¹⁵ N nuclear magnetic shielding scale from gas phase studies. Journal of Chemical Physics, 1981, 74, 81-88.	3.0	179
4	Gas-phase NMR spectroscopy. Chemical Reviews, 1991, 91, 1375-1395.	47.7	175
5	Absolute shielding scale for ³¹ P from gas-phase NMR studies. Chemical Physics Letters, 1990, 167, 575-582.	2.6	168
6	Temperature and density dependence of ¹²⁹ Xe chemical shift in xenon gas. Journal of Chemical Physics, 1973, 59, 4540-4546.	3.0	156
7	Molecular electronic property density functions: The nuclear magnetic shielding density. Journal of Chemical Physics, 1980, 73, 5684-5692.	3.0	121
8	¹⁹ F nuclear magnetic shielding scale from gas phase studies. Journal of Chemical Physics, 1980, 73, 6013-6020.	3.0	120
9	Theoretical Aspects of Isotope Effects on Nuclear Shielding. Annual Reports on NMR Spectroscopy, 1986, , 1-78.	1.5	106
10	Systematic Trends in the Coupling Constants of Directly Bonded Nuclei. Journal of Chemical Physics, 1969, 51, 2790-2803.	3.0	103
11	Grand canonical Monte Carlo simulations of the distribution and chemical shifts of xenon in the cages of zeolite NaA. I. Distribution and ¹²⁹ Xe chemical shifts. Journal of Chemical Physics, 1994, 100, 5965-5976.	3.0	103
12	The isotope shift in NMR. Journal of Chemical Physics, 1977, 66, 4983-4988.	3.0	101
13	UNDERSTANDING NMR CHEMICAL SHIFTS. Annual Review of Physical Chemistry, 1996, 47, 135-169.	10.8	101
14	Nuclear magnetic resonance studies of xenon clusters in zeolite NaA. Journal of Chemical Physics, 1992, 96, 1676-1689.	3.0	97
15	Abinitio calculations of the intermolecular chemical shift in nuclear magnetic resonance in the gas phase and for adsorbed species. Journal of Chemical Physics, 1992, 97, 417-434.	3.0	97
16	Nuclear spin relaxation by intermolecular magnetic dipole coupling in the gas phase. ¹²⁹ Xe in oxygen. Journal of Chemical Physics, 1988, 89, 4074-4081.	3.0	89
17	Competitive adsorption of xenon and krypton in zeolite NaA: ¹²⁹ Xe nuclear magnetic resonance studies and grand canonical Monte Carlo simulations. Journal of Chemical Physics, 1997, 107, 4364-4372.	3.0	88
18	Variation of chemical shielding with internal coordinates. Applications to diatomic molecules. Journal of Chemical Physics, 1977, 66, 4977-4982.	3.0	73

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19	Temperature and density dependence of ^{129}Xe chemical shift in rare gas mixtures. <i>Journal of Chemical Physics</i> , 1975, 62, 4224-4226.	3.0	70
20	Abinitio study of van der Waals interaction of CO_2 with Ar. <i>Journal of Chemical Physics</i> , 1996, 104, 6569-6576.	3.0	70
21	Xe nuclear magnetic resonance line shapes in nanochannels. <i>Journal of Chemical Physics</i> , 2002, 116, 3805-3821.	3.0	67
22	Nuclear magnetic shielding density. <i>The Journal of Physical Chemistry</i> , 1979, 83, 3366-3371.	2.9	66
23	The ^{31}P shielding in phosphine. <i>Journal of Chemical Physics</i> , 1991, 95, 9042-9053.	3.0	65
24	Isotope and temperature dependence of transition-metal shielding in complexes of the type $\text{M}(\text{XY})_6$. <i>Journal of the American Chemical Society</i> , 1987, 109, 2589-2594.	13.7	64
25	Xe NMR lineshapes in channels of peptide molecular crystals. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 17924-17929.	7.1	63
26	Spin-Spin Coupling. , 1987, , 89-131.		59
27	An abinitio study of the molecular electric polarizabilities of N_2 , HCN, acetylene, and diacetylene. <i>Journal of Chemical Physics</i> , 1986, 85, 3432-3436.	3.0	58
28	Grand canonical Monte Carlo simulations of the distribution and chemical shifts of xenon in the cages of zeolite NaA. II. Structure of the adsorbed fluid. <i>Journal of Chemical Physics</i> , 1994, 100, 5977-5987.	3.0	58
29	Nuclear magnetic shielding of nitrogen in ammonia. <i>Journal of Chemical Physics</i> , 1991, 95, 1069-1079.	3.0	57
30	Isotope effects on spin-spin coupling. <i>Journal of the American Chemical Society</i> , 1986, 108, 2497-2503.	13.7	55
31	Concurrent ^{19}F and ^{77}Se or ^{19}F and ^{125}Te NMR T_1 measurements for determination of ^{77}Se and ^{125}Te absolute shielding scales. <i>Chemical Physics Letters</i> , 1987, 135, 254-259.	2.6	53
32	Ion permeation dynamics in carbon nanotubes. <i>Journal of Chemical Physics</i> , 2006, 125, 084713.	3.0	52
33	^{19}F nuclear magnetic shielding scale from gas phase studies. II. <i>Journal of Chemical Physics</i> , 1984, 81, 5266-5267.	3.0	50
34	The NMR Chemical Shift: Insight into Structure and Environment. <i>Annual Reports on NMR Spectroscopy</i> , 1994, 29, 1-69.	1.5	50
35	Anisotropic Xe Chemical Shifts in Zeolites. The Role of Intra- and Intercrystallite Diffusion. <i>Journal of Physical Chemistry B</i> , 1997, 101, 8418-8437.	2.6	50
36	The Chemical Shift. , 1987, , 51-88.		50

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37	Absolute shielding scale for ^{29}Si . <i>Chemical Physics Letters</i> , 1988, 149, 300-305.	2.6	48
38	The nuclear magnetic shielding as a function of internuclear separation. <i>Journal of Chemical Physics</i> , 1993, 98, 2208-2217.	3.0	48
39	The additivity of NMR isotope shifts. <i>Journal of Chemical Physics</i> , 1984, 81, 4293-4299.	3.0	47
40	Temperature dependence of the ^{15}N and ^1H nuclear magnetic shielding in NH_3 . <i>Journal of Chemical Physics</i> , 1981, 74, 1608-1612.	3.0	43
41	Cage migration rates of Xe atoms in zeolite NaA from magnetization transfer experiments and simulations. <i>Journal of Chemical Physics</i> , 1994, 101, 1775-1786.	3.0	43
42	Competitive adsorption of xenon and argon in zeolite NaA. ^{129}Xe nuclear magnetic resonance studies and grand canonical Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 1996, 104, 1709-1728.	3.0	41
43	Molecular dynamics simulation of ion selectivity process in nanopores. <i>Molecular Simulation</i> , 2008, 34, 169-175.	2.0	40
44	Signs of 1KPC and other coupling constants in phosphorus and selenium compounds. <i>Journal of the American Chemical Society</i> , 1969, 91, 6232-6234.	13.7	39
45	Dependence of ^{19}F chemical shielding on internal coordinates in CF_4 , SiF_4 , and BF_3 . <i>Journal of Chemical Physics</i> , 1977, 67, 2814.	3.0	39
46	Theoretical calculations of the Xe chemical shifts in cryptophane cages. <i>Journal of Chemical Physics</i> , 2003, 119, 12231-12244.	3.0	39
47	Nanoparticle Permeation Induces Water Penetration, Ion Transport, and Lipid Flip-Flop. <i>Langmuir</i> , 2012, 28, 16989-17000.	3.5	39
48	On the spin-spin coupling between ^{13}C and H separated by two bonds. <i>Molecular Physics</i> , 1970, 18, 491-504.	1.7	38
49	The NMR isotope shift in polyatomic molecules. Estimation of the dynamic factors. <i>Journal of Chemical Physics</i> , 1984, 81, 4300-4305.	3.0	38
50	Variation of chemical shielding with intermolecular interactions and rovibrational motion. I. ^{19}F nuclei in BF_3 , CF_4 , SiF_4 , and SF_6 . <i>Journal of Chemical Physics</i> , 1977, 67, 2771.	3.0	37
51	The dependence of the ^{13}C and the ^1H nuclear magnetic shielding on bond extension in methane. <i>Journal of Chemical Physics</i> , 1984, 81, 4288-4292.	3.0	36
52	Variation of chemical shielding with intermolecular interaction and rovibrational motion. V. ^{15}N in N_2 . <i>Journal of Chemical Physics</i> , 1981, 74, 853-856.	3.0	35
53	A comparative study of CO_2 -Ar potential surfaces. <i>Journal of Chemical Physics</i> , 1996, 105, 6787-6806.	3.0	34
54	The ^{129}Xe nuclear shielding tensor surfaces for Xe interacting with rare gas atoms. <i>Journal of Chemical Physics</i> , 2003, 118, 2575.	3.0	34

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55	The nuclear magnetic resonance line shapes of Xe in the cages of clathrate hydrates. <i>Journal of Chemical Physics</i> , 2004, 120, 10200-10214.	3.0	34
56	Diastereomeric Xe Chemical Shifts in Tethered Cryptophane Cages. <i>Journal of the American Chemical Society</i> , 2006, 128, 16980-16988.	13.7	34
57	Absolute temperature dependence of chemical shifts of lock solvents. Tetramethylsilane, hexafluorobenzene, and 1,4-dibromotetrafluorobenzene. <i>Journal of the American Chemical Society</i> , 1973, 95, 8559-8561.	13.7	33
58	An empirical chemical shielding function for interacting atoms from direct inversion of NMR data. <i>Journal of Chemical Physics</i> , 1975, 63, 5296-5301.	3.0	33
59	Calculations of Xe line shapes in model nanochannels: Grand canonical Monte Carlo averaging of the ^{129}Xe nuclear magnetic resonance chemical shift tensor. <i>Journal of Chemical Physics</i> , 2002, 116, 8912-8929.	3.0	33
60	The chemical shifts of Xe in the cages of clathrate hydrate Structures I and II. <i>Journal of Chemical Physics</i> , 2004, 120, 1560-1571.	3.0	33
61	Permeation of nanocrystals across lipid membranes. <i>Molecular Physics</i> , 2011, 109, 1511-1526.	1.7	33
62	Role of surface ligands in nanoparticle permeation through a model membrane: a coarse-grained molecular dynamics simulations study. <i>Molecular Physics</i> , 2012, 110, 2181-2195.	1.7	33
63	Surface-Functionalized Nanoparticle Permeation Triggers Lipid Displacement and Water and Ion Leakage. <i>Langmuir</i> , 2015, 31, 1074-1085.	3.5	33
64	The ^{129}Xe nuclear shielding surfaces for Xe interacting with linear molecules CO_2 , N_2 , and CO . <i>Journal of Chemical Physics</i> , 1997, 107, 4253-4270.	3.0	32
65	Variation of chemical shielding with intermolecular interactions and rovibrational motion. IV. ^{11}B and ^{13}C nuclei in BF_3 and CH_4 . <i>Journal of Chemical Physics</i> , 1978, 68, 2873.	3.0	31
66	^{129}Xe nuclear magnetic resonance studies of xenon in zeolite CaA. <i>Journal of Chemical Physics</i> , 1992, 96, 1690-1697.	3.0	31
67	Reply to `conventions for tensor quantities used in nuclear magnetic resonance, nuclear quadrupole resonance and electron spin resonance spectroscopy. <i>Solid State Nuclear Magnetic Resonance</i> , 1998, 11, 265-268.	2.3	31
68	Molecular dynamics averaging of Xe chemical shifts in liquids. <i>Journal of Chemical Physics</i> , 2004, 121, 9581-9592.	3.0	30
69	^{15}N spin-relaxation studies of N_2 in buffer gases. Cross sections for molecular reorientation and rotational energy transfer. <i>Journal of Chemical Physics</i> , 1987, 86, 6833-6838.	3.0	29
70	Isotope effects on proton chemical shifts and coupling constants in the ammonium ions ^{15}N , ^{14}N . <i>Chemical Physics Letters</i> , 1988, 143, 471-476.	2.6	29
71	^{129}Xe Magic-angle spinning spectra of xenon in zeolite NaA direct observation of mixed clusters of co-adsorbed species. <i>Solid State Nuclear Magnetic Resonance</i> , 1995, 4, 1-12.	2.3	29
72	A note on chirality in NMR spectroscopy. <i>Journal of Chemical Physics</i> , 2006, 124, 096101.	3.0	29

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73	Variation of chemical shielding with intermolecular interactions and rovibrational motion. II. ^{15}N and ^{13}C nuclei in N_2O and CO_2 . <i>Journal of Chemical Physics</i> , 1978, 68, 2861.	3.0	28
74	Correlation between the ^{19}F absolute nuclear magnetic shielding and its temperature dependence in the fluoromethanes. <i>Molecular Physics</i> , 1985, 54, 73-79.	1.7	28
75	Systematic trends in the variation of ^{19}F nuclear magnetic shielding with bond extension in halomethanes. <i>Molecular Physics</i> , 1985, 55, 383-395.	1.7	28
76	Density dependence of ^{129}Xe N.M.R. chemical shifts in O_2 and NO . <i>Molecular Physics</i> , 1971, 20, 957-959.	1.7	27
77	Second virial coefficient of ^{129}Xe chemical shielding in mixtures of Xe with spherical top molecules CH_4 , CF_4 , and SiF_4 . <i>Journal of Chemical Physics</i> , 1976, 65, 3401-3406.	3.0	27
78	Cross sections for transfer of rotational angular momentum in CO_2 from ^{13}C spin relaxation studies in the gas phase. <i>Journal of Chemical Physics</i> , 1987, 86, 2717-2722.	3.0	27
79	Transport of Vanadium and Oxovanadium Ions Across Zeolite Membranes: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 23803-23810.	3.1	27
80	The temperature dependence of chemical shielding in diatomic molecules: CO , F_2 , ClF , HBr , and HCl . <i>Journal of Chemical Physics</i> , 1977, 67, 2821.	3.0	26
81	Carbon-13 and proton spin relaxation in methane in the gas phase. <i>The Journal of Physical Chemistry</i> , 1991, 95, 1092-1098.	2.9	26
82	Xen clusters in the alpha cages of zeolite KA. <i>Journal of Chemical Physics</i> , 1995, 103, 8811-8820.	3.0	26
83	^{14}N spin relaxation studies of N_2 in buffer gases. Cross sections for molecular reorientation and rotational energy transfer. <i>Journal of Chemical Physics</i> , 1991, 95, 5799-5808.	3.0	25
84	Molecular dynamics simulations of the chiral recognition mechanism for a polysaccharide chiral stationary phase in enantiomeric chromatographic separations. <i>Molecular Physics</i> , 2019, 117, 3569-3588.	1.7	25
85	Applications of the reduced isotope shift to general estimation of one-bond isotope shifts in NMR. <i>Journal of the American Chemical Society</i> , 1985, 107, 4158-4161.	13.7	24
86	Intermolecular effects on ^1H , ^{13}C , and ^{15}N nuclear magnetic shielding in HCN . <i>Journal of Chemical Physics</i> , 1982, 76, 152-162.	3.0	23
87	The effect of anharmonic vibration and centrifugal distortion on nuclear shielding in linear triatomic molecules: N_2O and CO_2 . <i>Journal of Chemical Physics</i> , 1984, 81, 2556-2561.	3.0	23
88	Rovibrational effects on nuclear shielding of apex nuclei in bent molecules. <i>Journal of Chemical Physics</i> , 1985, 82, 4595-4606.	3.0	23
89	Modeling Enantiomeric Separations as an Interfacial Process Using Amylose Tris(3,5-dimethylphenyl) Tj ETQq1 1 0.784314 rgBT /Over	3.5	23
90	Absolute temperature dependence of chemical shielding of some reference nuclei. <i>Journal of Magnetic Resonance</i> , 1975, 19, 385-392.	0.5	22

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91	Effects of intermolecular interactions and intramolecular dynamics on nuclear resonance in nitrogen trifluoride, phosphorus trifluoride, phosphoryl fluoride, and phosphorus pentafluoride. <i>The Journal of Physical Chemistry</i> , 1979, 83, 3372-3378.	2.9	22
92	Temperature dependence of ^{77}Se , ^{125}Te , and ^{19}F shielding and M -induced ^{19}F isotope shifts in MF_6 molecules. <i>Journal of Chemical Physics</i> , 1986, 85, 5480-5483.	3.0	22
93	Deuterium-induced ^{19}F isotope shifts in fluoroethenes. <i>Journal of Chemical Physics</i> , 1985, 83, 5434-5441.	3.0	21
94	Simulated Permeation and Characterization of PEGylated Gold Nanoparticles in a Lipid Bilayer System. <i>Langmuir</i> , 2016, 32, 7541-7555.	3.5	21
95	^{129}Xe contact shift in oxygen gas. <i>Molecular Physics</i> , 1975, 29, 1919-1927.	1.7	20
96	Angular momentum relaxation in binary collisions. Comparison of cross sections. <i>Journal of Chemical Physics</i> , 1990, 93, 3237-3244.	3.0	20
97	Ab initio studies of the nuclear magnetic resonance chemical shifts of a rare gas atom in a zeolite. <i>Journal of Chemical Physics</i> , 1995, 103, 3885-3894.	3.0	20
98	Effect of interactions with nonspherical molecules on ^{129}Xe magnetic shielding. <i>Journal of Chemical Physics</i> , 1977, 66, 5226-5230.	3.0	19
99	^{19}F NMR chemical shifts due to intermolecular interactions in $\text{F}_2\text{C}=\text{CFX}$. A quantitative measure of the nuclear site effect. <i>Journal of Chemical Physics</i> , 1984, 81, 2313-2317.	3.0	19
100	Adsorption of xenon and CH_4 mixtures in zeolite NaA. ^{129}Xe NMR and grand canonical Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2000, 112, 323-334.	3.0	19
101	The Xe shielding surfaces for Xe interacting with linear molecules and spherical tops. <i>Journal of Chemical Physics</i> , 2004, 121, 2151-2157.	3.0	19
102	Recent Advances in Nuclear Shielding Calculations. <i>Annual Reports on NMR Spectroscopy</i> , 2012, 77, 1-80.	1.5	19
103	Second virial coefficient of ^{129}Xe chemical shielding in Xe interacting with CO and N_2 molecules. <i>Journal of Chemical Physics</i> , 1978, 68, 3943-3944.	3.0	18
104	Classical trajectories on simple model potentials for $\text{N}_2\text{-Kr}$: Comparison with relaxation and other data. <i>Journal of Chemical Physics</i> , 1995, 102, 4431-4446.	3.0	18
105	Calculation of the ^{129}Xe chemical shift in $\text{Xe}@C_{60}$. <i>Journal of Chemical Physics</i> , 2003, 118, 9987-9989.	3.0	18
106	Variation of nuclear magnetic shielding with intermolecular interactions and rovibrational motion. VII. ^{19}F in CF_2H_2 , CF_2HCl , CFHCl_2 , CF_2Cl_2 , and CFCl_3 . <i>Journal of Chemical Physics</i> , 1984, 81, 85-90.	3.0	17
107	Rovibrational averaging of molecular magnetic properties of CH_3F , CH_2F_2 , and CHF_3 . <i>Molecular Physics</i> , 1985, 56, 1083-1095.	1.7	17
108	Rovibrational averaging of nuclear shielding in MX_6 -type molecules. <i>Journal of Chemical Physics</i> , 1986, 85, 5484-5492.	3.0	17

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109	Effective collision cross sections for SF ₆ from nuclear magnetic relaxation. Journal of Chemical Physics, 1988, 88, 7448-7452.	3.0	17
110	Nuclear magnetic shielding and chirality IV. The odd and even character of the shielding response to a chiral potential. Journal of Chemical Physics, 2004, 120, 3277-3283.	3.0	17
111	Computational Molecular Modeling of Transport Processes in Nanoporous Membranes. Processes, 2018, 6, 124.	2.8	17
112	Contact interaction between ¹²⁹ Xe and nitric oxide. Journal of Chemical Physics, 1976, 65, 3397-3400.	3.0	16
113	N ₂ -Kr interaction: A multiproperty analysis. Journal of Chemical Physics, 1995, 102, 5752-5760.	3.0	16
114	Distribution and ¹²⁹ Xe NMR chemical shifts of Xen clusters in the alpha cages of zeolite AgA. Journal of Chemical Physics, 1997, 107, 4373-4383.	3.0	16
115	Xe Chemical Shift Tensor in Silicalite and SSZ-24. Journal of the American Chemical Society, 2004, 126, 10450-10456.	13.7	16
116	Exploring gas permeability of lipid membranes using coarse-grained molecular dynamics. Molecular Simulation, 2009, 35, 953-961.	2.0	16
117	The Nuclear Shielding Surface: The Shielding as a Function of Molecular Geometry and Intermolecular Separation. , 1993, , 95-116.		16
118	The mean bond displacements and the derivatives of ¹⁹ F shielding in CF ₂ =CFX and CF ₂ =CH ₂ . Journal of Chemical Physics, 1985, 83, 5425-5433.	3.0	15
119	Gas-liquid shifts in NMR and the validity of the second virial coefficient of chemical shielding. Journal of Chemical Physics, 1979, 70, 5916-5917.	3.0	14
120	The role of polarization of Xe by di- and monovalent cations in ¹²⁹ Xe NMR studies in zeolite A. Solid State Nuclear Magnetic Resonance, 1997, 9, 277-301.	2.3	14
121	Quantum-mechanical treatment of the electronic structure and geometry of hydrogen cyanide dimer. Journal of Theoretical Biology, 1972, 35, 247-257.	1.7	13
122	Variation of chemical shielding with intermolecular interactions and rovibrational motion. III. ³¹ P nucleus in PH ₃ . Journal of Chemical Physics, 1978, 68, 2868.	3.0	13
123	Effects of rovibrational averaging on the niobium-93 chemical shift in the hexacarbonylniobate(1-) ion, based on NMR and vibrational spectra. Inorganic Chemistry, 1988, 27, 3490-3495.	4.0	13
124	Cross sections for the anisotropic interaction of NNO with various molecules. Journal of Chemical Physics, 1988, 89, 5642-5649.	3.0	13
125	Rotational behaviour of PEGylated gold nanorods in a lipid bilayer system. Molecular Physics, 2017, 115, 1122-1143.	1.7	13
126	Isotope effects in ³¹ P NMR of phosphine. Journal of Magnetic Resonance, 1978, 32, 455-457.	0.5	12

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127	Effect of centrifugal distortion and anharmonic vibration on the ^{19}F chemical shielding in CH_3F . Journal of Chemical Physics, 1978, 69, 1655-1660.	3.0	12
128	Temperature dependence of the chemical shielding of ^{19}F nuclei in isolated CF_3H , CF_3Cl , CF_3Br , and CF_3CF_3 molecules. Journal of Chemical Physics, 1978, 69, 1318.	3.0	12
129	The mean bond displacements in $\text{O}=\text{CF}_2$ and their effect on ^{19}F nuclear magnetic shielding. Journal of Chemical Physics, 1984, 81, 4915-4921.	3.0	12
130	Nuclear spin relaxation studies of the spin-rotation interaction of ^{13}C in CO in various buffer gases. Journal of Chemical Physics, 1986, 85, 697-700.	3.0	12
131	Molecular Dynamics Simulations of Xe Chemical Shifts and Solubility in <i>n</i> -Alkanes. Journal of Physical Chemistry C, 2007, 111, 15771-15783.	3.1	12
132	Measuring chirality in NMR in the presence of a static electric field. Journal of Chemical Physics, 2008, 128, 154502.	3.0	12
133	Diffusion of gases across lipid membranes with OmpA channel: a molecular dynamics study. Molecular Physics, 2010, 108, 1569-1581.	1.7	12
134	Variation of nuclear magnetic shielding with intermolecular interactions and rovibrational motion. IX. ^{19}F in $\text{F}_2\text{C}=\text{CH}_2$ and $\text{F}_2\text{C}=\text{CF}_2$. Journal of Chemical Physics, 1984, 81, 2571-2573.	3.0	11
135	Variation of nuclear magnetic shielding with intermolecular interactions and rovibrational motion. VIII. ^{19}F in CF_3X . Journal of Chemical Physics, 1984, 81, 1198-1202.	3.0	11
136	Quadrupolar spin relaxation due to electric field gradients induced by vibrations and collisions. Molecular Physics, 1986, 57, 553-571.	1.7	11
137	Nuclear magnetic shielding and chirality. I. The shielding tensor of Xe interacting with Ne helices. Journal of Chemical Physics, 2003, 119, 2685-2690.	3.0	11
138	Vibrational analysis and mean bond displacements in $\text{M}(\text{XY})_6$ complexes. Journal of the American Chemical Society, 1987, 109, 2586-2588.	13.7	10
139	Molecular dynamics simulations reveal how characteristics of surface and permeant affect permeation events at the surface of soft matter. Molecular Simulation, 2017, 43, 439-466.	2.0	10
140	The Parameters of NMR Spectroscopy. , 1987, , 3-50.		10
141	Relaxation cross sections for the rotational angular momentum vector in CF_4 . Journal of Chemical Physics, 1988, 89, 866-870.	3.0	9
142	Nuclear magnetic shielding and chirality. III. The single electron on a helix model. Journal of Chemical Physics, 2003, 119, 2694-2701.	3.0	8
143	Prediction of Henry's constants of xenon in cyclo-alkanes from molecular dynamics simulations. Fluid Phase Equilibria, 2008, 269, 73-79.	2.5	8
144	Molecular dynamics simulations of enantiomeric separations as an interfacial process in $\langle \text{scp} \rangle \text{HPLC} \langle / \text{scp} \rangle$. AIChE Journal, 2021, 67, e17143.	3.6	8

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145	Rovibrational Averaging of Molecular Electronic Properties. , 1991, , 457-519.		8
146	Effects of vibrational anharmonicity on ^{19}F nuclear resonance in SF_6 . Molecular Physics, 1980, 40, 999-1003.	1.7	7
147	Nuclear magnetic shielding and chirality. II. The shielding tensor of a naked spin in Ne helices. Journal of Chemical Physics, 2003, 119, 2691-2693.	3.0	7
148	Xe nuclear magnetic resonance line shapes in channels decorated with paramagnetic centers. Journal of Chemical Physics, 2006, 125, 114708.	3.0	7
149	Using Molecular Simulations To Develop Reliable Design Tools and Correlations for Engineering Applications of Aqueous Electrolyte Solutions. Journal of Chemical & Engineering Data, 2016, 61, 1578-1584.	1.9	7
150	Fluorine. , 1987, , 437-446.		7
151	Theoretical and physical aspects of nuclear shielding. Nuclear Magnetic Resonance, 0, , 42-76.	0.2	7
152	Variation of chemical shielding with intermolecular interactions and rovibrational motion. VI. ^{19}F in SF_4 and COF_2 . Journal of Chemical Physics, 1981, 74, 1613-1617.	3.0	6
153	^{19}F nuclear spin relaxation by intermolecular magnetic dipole coupling. CF_4 and SiF_4 in oxygen gas. Journal of Chemical Physics, 1991, 94, 172-178.	3.0	6
154	On using the NMR chemical shift to assess polar vs nonpolar cross-intermolecular interactions. Chemical Physics Letters, 2003, 380, 556-562.	2.6	6
155	Intermolecular hyperfine tensor for $\text{Xe}@\text{O}_2$. Density and temperature dependence of Xe chemical shifts in oxygen gas. Molecular Physics, 2006, 104, 1217-1225.	1.7	6
156	Theoretical and physical aspects of nuclear shielding. Nuclear Magnetic Resonance, 2015, , 46-75.	0.2	6
157	Effect of centrifugal distortion and anharmonic vibration on the chemical shielding of ^{31}P in PH_3 and PD_3 . Journal of Chemical Physics, 1978, 69, 615-621.	3.0	5
158	Variation of nuclear magnetic shielding of ^{19}F with intermolecular interactions and rovibrational motion in fluoroethanes. Journal of Magnetic Resonance, 1985, 62, 209-217.	0.5	5
159	Competition of intra- and intermolecular spin relaxation mechanisms for SF_6 in oxygen gas. The Journal of Physical Chemistry, 1988, 92, 5937-5941.	2.9	5
160	Proton relaxation in methane with oxygen gas. The Journal of Physical Chemistry, 1989, 93, 634-638.	2.9	5
161	Deuterium isotope effects and bonding in carbonylvanadium complexes. Magnetic Resonance in Chemistry, 1990, 28, 138-144.	1.9	5
162	Quadrupolar spin relaxation of ^{14}N in NNO in collisions with various molecules. Journal of Chemical Physics, 1998, 109, 10227-10237.	3.0	5

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163	Molecular dynamics simulations of chiral recognition of drugs by amylose polymers coated on amorphous silica. <i>Molecular Physics</i> , 2021, 119, .	1.7	5
164	Theoretical and physical aspects of nuclear shielding. <i>Nuclear Magnetic Resonance</i> , 0, , 1-17.	0.2	5
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