Cynthia J Jameson

List of Publications by Year
in descending order

185 papers	6,281 citations	81743 39 h-index	95083 68 g-index
200 all docs	200 docs citations	200 times ranked	2505 citing authors

#	Article	IF	Citations
1	Gas-phase 13C chemical shifts in the zero-pressure limit: refinements to the absolute shielding scale for 13C. Chemical Physics Letters, 1987, 134, 461-466.	1.2	398
2	Density Dependence of 129Xe Chemical Shifts in Mixtures of Xenon and Other Gases. Journal of Chemical Physics, 1970, 53, 2310-2321.	1.2	189
3	15N nuclear magnetic shielding scale from gas phase studies. Journal of Chemical Physics, 1981, 74, 81-88.	1.2	179
4	Gas-phase NMR spectroscopy. Chemical Reviews, 1991, 91, 1375-1395.	23.0	175
5	Absolute shielding scale for 31P from gas-phase NMR studies. Chemical Physics Letters, 1990, 167, 575-582.	1.2	168
6	Temperature and density dependence of 129Xe chemical shift in xenon gas. Journal of Chemical Physics, 1973, 59, 4540-4546.	1.2	156
7	Molecular electronic property density functions: The nuclear magnetic shielding density. Journal of Chemical Physics, 1980, 73, 5684-5692.	1.2	121
8	19F nuclear magnetic shielding scale from gas phase studies. Journal of Chemical Physics, 1980, 73, 6013-6020.	1.2	120
9	Theoretical Aspects of Isotope Effects on Nuclear Shielding. Annual Reports on NMR Spectroscopy, 1986, , 1-78.	0.7	106
10	Systematic Trends in the Coupling Constants of Directly Bonded Nuclei. Journal of Chemical Physics, 1969, 51, 2790-2803.	1.2	103
11	Grand canonical Monte Carlo simulations of the distribution and chemical shifts of xenon in the cages of zeolite NaA. I. Distribution and 129Xe chemical shifts. Journal of Chemical Physics, 1994, 100, 5965-5976.	1.2	103
12	The isotope shift in NMR. Journal of Chemical Physics, 1977, 66, 4983-4988.	1.2	101
13	UNDERSTANDING NMR CHEMICAL SHIFTS. Annual Review of Physical Chemistry, 1996, 47, 135-169.	4.8	101
14	Nuclear magnetic resonance studies of xenon clusters in zeolite NaA. Journal of Chemical Physics, 1992, 96, 1676-1689.	1.2	97
15	Abinitiocalculations 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.	1.2	97
16	Nuclear spin relaxation by intermolecular magnetic dipole coupling in the gas phase.129Xe in oxygen. Journal of Chemical Physics, 1988, 89, 4074-4081.	1.2	89
17	Competitive adsorption of xenon and krypton in zeolite NaA: 129Xe nuclear magnetic resonance studies and grand canonical Monte Carlo simulations. Journal of Chemical Physics, 1997, 107, 4364-4372.	1.2	88
18	Variation of chemical shielding with internal coordinates. Applications to diatomic molecules. Journal of Chemical Physics, 1977, 66, 4977-4982.	1.2	73

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19	Temperature and density dependence of 129Xe chemical shift in rare gas mixtures. Journal of Chemical Physics, 1975, 62, 4224-4226.	1.2	70
20	Abinitiostudy of van der Waals interaction of CO2with Ar. Journal of Chemical Physics, 1996, 104, 6569-6576.	1.2	70
21	Xe nuclear magnetic resonance line shapes in nanochannels. Journal of Chemical Physics, 2002, 116, 3805-3821.	1.2	67
22	Nuclear magnetic shielding density. The Journal of Physical Chemistry, 1979, 83, 3366-3371.	2.9	66
23	The31P shielding in phosphine. Journal of Chemical Physics, 1991, 95, 9042-9053.	1.2	65
24	Isotope and temperature dependence of transition-metal shielding in complexes of the type M(XY)6. Journal of the American Chemical Society, 1987, 109, 2589-2594.	6.6	64
25	Xe NMR lineshapes in channels of peptide molecular crystals. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 17924-17929.	3.3	63
26	Spin-Spin Coupling. , 1987, , 89-131.		59
27	Anabinitiostudy of the molecular electric polarizabilities of N2, HCN, acetylene, and diacetylene. Journal of Chemical Physics, 1986, 85, 3432-3436.	1.2	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. Journal of Chemical Physics, 1994, 100, 5977-5987.	1.2	58
29	Nuclear magnetic shielding of nitrogen in ammonia. Journal of Chemical Physics, 1991, 95, 1069-1079.	1.2	57
30	Isotope effects on spin-spin coupling. Journal of the American Chemical Society, 1986, 108, 2497-2503.	6.6	55
31	Concurrent 19F and 77Se or 19F and 125Te NMR T1 measurements for determination of 77Se and 125Te absolute shielding scales. Chemical Physics Letters, 1987, 135, 254-259.	1.2	53
32	Ion permeation dynamics in carbon nanotubes. Journal of Chemical Physics, 2006, 125, 084713.	1.2	52
33	19F nuclear magnetic shielding scale from gas phase studies. II. Journal of Chemical Physics, 1984, 81, 5266-5267.	1.2	50
34	The NMR Chemical Shift: Insight into Structure and Environment. Annual Reports on NMR Spectroscopy, 1994, 29, 1-69.	0.7	50
35	Anisotropic Xe Chemical Shifts in Zeolites. The Role of Intra- and Intercrystallite Diffusion. Journal of Physical Chemistry B, 1997, 101, 8418-8437.	1.2	50
36	The Chemical Shift. , 1987, , 51-88.		50

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37	Absolute shielding scale for 29Si. Chemical Physics Letters, 1988, 149, 300-305.	1.2	48
38	The nuclear magnetic shielding as a function of internuclear separation. Journal of Chemical Physics, 1993, 98, 2208-2217.	1.2	48
39	The additivity of NMR isotope shifts. Journal of Chemical Physics, 1984, 81, 4293-4299.	1.2	47
40	Temperature dependence of the15N and1H nuclear magnetic shielding in NH3. Journal of Chemical Physics, 1981, 74, 1608-1612.	1.2	43
41	Cageâ€toâ€cage migration rates of Xe atoms in zeolite NaA from magnetization transfer experiments and simulations. Journal of Chemical Physics, 1994, 101, 1775-1786.	1.2	43
42	Competitive adsorption of xenon and argon in zeolite NaA. 129Xe nuclear magnetic resonance studies and grand canonical Monte Carlo simulations. Journal of Chemical Physics, 1996, 104, 1709-1728.	1.2	41
43	Molecular dynamics simulation of ion selectivity process in nanopores. Molecular Simulation, 2008, 34, 169-175.	0.9	40
44	Signs of 1KPC and other coupling constants in phosphorus and selenium compounds. Journal of the American Chemical Society, 1969, 91, 6232-6234.	6.6	39
45	Dependence of 19F chemical shielding on internal coordinates in CF4, SiF4, and BF3. Journal of Chemical Physics, 1977, 67, 2814.	1.2	39
46	Theoretical calculations of the Xe chemical shifts in cryptophane cages. Journal of Chemical Physics, 2003, 119, 12231-12244.	1.2	39
47	Nanoparticle Permeation Induces Water Penetration, Ion Transport, and Lipid Flip-Flop. Langmuir, 2012, 28, 16989-17000.	1.6	39
48	On the spin-spin coupling between13C and H separated by two bonds. Molecular Physics, 1970, 18, 491-504.	0.8	38
49	The NMR isotope shift in polyatomic molecules. Estimation of the dynamic factors. Journal of Chemical Physics, 1984, 81, 4300-4305.	1.2	38
50	Variation of chemical shielding with intermolecular interactions and rovibrational motion. I. 19F nuclei in BF3, CF4, SiF4, and SF6. Journal of Chemical Physics, 1977, 67, 2771.	1.2	37
51	The dependence of the13C and the1H nuclear magnetic shielding on bond extension in methane. Journal of Chemical Physics, 1984, 81, 4288-4292.	1.2	36
52	Variation of chemical shielding with intermolecular interaction and rovibrational motion. V.15N in N2. Journal of Chemical Physics, 1981, 74, 853-856.	1.2	35
53	A comparative study of CO2â€“Ar potential surfaces. Journal of Chemical Physics, 1996, 105, 6787-6806.	1.2	34
54	The [sup 129]Xe nuclear shielding tensor surfaces for Xe interacting with rare gas atoms. Journal of Chemical Physics, 2003, 118, 2575.	1.2	34

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55	The nuclear magnetic resonance line shapes of Xe in the cages of clathrate hydrates. Journal of Chemical Physics, 2004, 120, 10200-10214.	1.2	34
56	Diastereomeric Xe Chemical Shifts in Tethered Cryptophane Cages. Journal of the American Chemical Society, 2006, 128, 16980-16988.	6.6	34
57	Absolute temperature dependence of chemical shifts of lock solvents. Tetramethylsilane, hexafluorobenzene, and 1,4-dibromotetrafluorobenzene. Journal of the American Chemical Society, 1973, 95, 8559-8561.	6.6	33
58	An empirical chemical shielding function for interacting atoms from direct inversion of NMR data. Journal of Chemical Physics, 1975, 63, 5296-5301.	1.2	33
59	Calculations of Xe line shapes in model nanochannels: Grand canonical Monte Carlo averaging of the 129Xe nuclear magnetic resonance chemical shift tensor. Journal of Chemical Physics, 2002, 116, 8912-8929.	1.2	33
60	The chemical shifts of Xe in the cages of clathrate hydrate Structures I and II. Journal of Chemical Physics, 2004, 120, 1560-1571.	1.2	33
61	Permeation of nanocrystals across lipid membranes. Molecular Physics, 2011, 109, 1511-1526.	0.8	33
62	Role of surface ligands in nanoparticle permeation through a model membrane: a coarse-grained molecular dynamics simulations study. Molecular Physics, 2012, 110, 2181-2195.	0.8	33
63	Surface-Functionalized Nanoparticle Permeation Triggers Lipid Displacement and Water and Ion Leakage. Langmuir, 2015, 31, 1074-1085.	1.6	33
64	The129Xe nuclear shielding surfaces for Xe interacting with linear molecules CO2, N2, and CO. Journal of Chemical Physics, 1997, 107, 4253-4270.	1.2	32
65	Variation of chemical shielding with intermolecular interactions and rovibrational motion. IV. 11B and 13C nuclei in BF3 and CH4. Journal of Chemical Physics, 1978, 68, 2873.	1.2	31
66	129Xe nuclear magnetic resonance studies of xenon in zeolite CaA. Journal of Chemical Physics, 1992, 96, 1690-1697.	1.2	31
67	Reply to `conventions for tensor quantities used in nuclear magnetic resonance, nuclear quadrupole resonance and electron spin resonance spectroscopy. Solid State Nuclear Magnetic Resonance, 1998, 11, 265-268.	1.5	31
68	Molecular dynamics averaging of Xe chemical shifts in liquids. Journal of Chemical Physics, 2004, 121, 9581-9592.	1.2	30
69	15N spinâ€relaxation studies of N2in buffer gases. Cross sections for molecular reorientation and rotational energy transfer. Journal of Chemical Physics, 1987, 86, 6833-6838.	1.2	29
70	Isotope effects on proton chemical shifts and coupling constants in the ammonium ions 15, 14 NH4-nDn+. Chemical Physics Letters, 1988, 143, 471-476.	1.2	29
71	129Xe Magic-angle spinning spectra of xenon in zeolite NaA direct observation of mixed clusters of co-adsorbed species. Solid State Nuclear Magnetic Resonance, 1995, 4, 1-12.	1.5	29
72	A note on chirality in NMR spectroscopy. Journal of Chemical Physics, 2006, 124, 096101.	1.2	29

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73	Variation of chemical shielding with intermolecular interactions and rovibrational motion. II. 15N and 13C nuclei in NNO and CO2. Journal of Chemical Physics, 1978, 68, 2861.	1.2	28
74	Correlation between the19F absolute nuclear magnetic shielding and its temperature dependence in the fluoromethanes. Molecular Physics, 1985, 54, 73-79.	0.8	28
75	Systematic trends in the variation of19F nuclear magnetic shielding with bond extension in halomethanes. Molecular Physics, 1985, 55, 383-395.	0.8	28
76	Density dependence of129Xe N.M.R. chemical shifts in O2and NO. Molecular Physics, 1971, 20, 957-959.	0.8	27
77	Second virial coefficient of129Xe chemical shielding in mixtures of Xe with spherical top molecules CH4, CF4, and SiF4. Journal of Chemical Physics, 1976, 65, 3401-3406.	1.2	27
78	Cross sections for transfer of rotational angular momentum in CO2from13C spin relaxation studies in the gas phase. Journal of Chemical Physics, 1987, 86, 2717-2722.	1.2	27
79	Transport of Vanadium and Oxovanadium Ions Across Zeolite Membranes: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2014, 118, 23803-23810.	1.5	27
80	The temperature dependence of chemical shielding in diatomic molecules: CO, F2, ClF, HBr, and HCl. Journal of Chemical Physics, 1977, 67, 2821.	1.2	26
81	Carbon-13 and proton spin relaxation in methane in the gas phase. The Journal of Physical Chemistry, 1991, 95, 1092-1098.	2.9	26
82	Xen clusters in the alpha cages of zeolite KA. Journal of Chemical Physics, 1995, 103, 8811-8820.	1.2	26
83	14N spin relaxation studies of N2in buffer gases. Cross sections for molecular reorientation and rotational energy transfer. Journal of Chemical Physics, 1991, 95, 5799-5808.	1.2	25
84	Molecular dynamics simulations of the chiral recognition mechanism for a polysaccharide chiral stationary phase in enantiomeric chromatographic separations. Molecular Physics, 2019, 117, 3569-3588.	0.8	25
85	Applications of the reduced isotope shift to general estimation of one-bond isotope shifts in NMR. Journal of the American Chemical Society, 1985, 107, 4158-4161.	6.6	24
86	Intermolecular effects on1H,13C, and15N nuclear magnetic shielding in HCN. Journal of Chemical Physics, 1982, 76, 152-162.	1.2	23
87	The effect of anharmonic vibration and centrifugal distortion on nuclear shielding in linear triatomic molecules: NNO and CO2. Journal of Chemical Physics, 1984, 81, 2556-2561.	1.2	23
88	Rovibrational effects on nuclear shielding of apex nuclei in bent molecules. Journal of Chemical Physics, 1985, 82, 4595-4606.	1.2	23
89	Modeling Enantiomeric Separations as an Interfacial Process Using Amylose Tris(3,5-dimethylphenyl) Tj ETQq1 1 0.784314 rgBT /Over	1.6	23
90	Absolute temperature dependence of chemical shielding of some reference nuclei. Journal of Magnetic Resonance, 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. The Journal of Physical Chemistry, 1979, 83, 3372-3378.	2.9	22
92	Temperature dependence of77Se,125Te, and19F shielding and Mâ€induced19F isotope shifts in MF6molecules. Journal of Chemical Physics, 1986, 85, 5480-5483.	1.2	22
93	Deuteriumâ€induced 19F isotope shifts in fluoroethenes. Journal of Chemical Physics, 1985, 83, 5434-5441.	1.2	21
94	Simulated Permeation and Characterization of PEGylated Gold Nanoparticles in a Lipid Bilayer System. Langmuir, 2016, 32, 7541-7555.	1.6	21
95	129Xe contact shift in oxygen gas. Molecular Physics, 1975, 29, 1919-1927.	0.8	20
96	Angular momentum relaxation in binary collisions. Comparison of cross sections. Journal of Chemical Physics, 1990, 93, 3237-3244.	1.2	20
97	Ab initiostudies of the nuclear magnetic resonance chemical shifts of a rare gas atom in a zeolite. Journal of Chemical Physics, 1995, 103, 3885-3894.	1.2	20
98	Effect of interactions with nonspherical molecules on129Xe magnetic shielding. Journal of Chemical Physics, 1977, 66, 5226-5230.	1.2	19
99	19F NMR chemical shifts due to intermolecular interactions in F2C=CFX. A quantitative measure of the nuclear site effect. Journal of Chemical Physics, 1984, 81, 2313-2317.	1.2	19
100	Adsorption of xenon and CH4 mixtures in zeolite NaA. 129Xe NMR and grand canonical Monte Carlo simulations. Journal of Chemical Physics, 2000, 112, 323-334.	1.2	19
101	The Xe shielding surfaces for Xe interacting with linear molecules and spherical tops. Journal of Chemical Physics, 2004, 121, 2151-2157.	1.2	19
102	Recent Advances in Nuclear Shielding Calculations. Annual Reports on NMR Spectroscopy, 2012, 77, 1-80.	0.7	19
103	Second virial coefficient of 129Xe chemical shielding in Xe interacting with CO and N2 molecules. Journal of Chemical Physics, 1978, 68, 3943-3944.	1.2	18
104	Classical trajectories on simple model potentials for N2â€“Kr: Comparison with relaxation and other data. Journal of Chemical Physics, 1995, 102, 4431-4446.	1.2	18
105	Calculation of the 129Xe chemical shift in Xe@C60. Journal of Chemical Physics, 2003, 118, 9987-9989.	1.2	18
106	Variation of nuclear magnetic shielding with intermolecular interactions and rovibrational motion. VII. 19F in CF2H2, CF2HCl, CFHCl2, CF2Cl2, and CFCl3. Journal of Chemical Physics, 1984, 81, 85-90.	1.2	17
107	Rovibrational averaging of molecular magnetic properties of CH3F, CH2F2, and CHF3. Molecular Physics, 1985, 56, 1083-1095.	0.8	17
108	Rovibrational averaging of nuclear shielding in MX6â€type molecules. Journal of Chemical Physics, 1986, 85, 5484-5492.	1.2	17

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109	Effective collision cross sections for SF6from nuclear magnetic relaxation. Journal of Chemical Physics, 1988, 88, 7448-7452.	1.2	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.	1.2	17
111	Computational Molecular Modeling of Transport Processes in Nanoporous Membranes. Processes, 2018, 6, 124.	1.3	17
112	Contact interaction between129Xe and nitric oxide. Journal of Chemical Physics, 1976, 65, 3397-3400.	1.2	16
113	N2â€“Kr interaction: A multiproperty analysis. Journal of Chemical Physics, 1995, 102, 5752-5760.	1.2	16
114	Distribution and Xe129 NMR chemical shifts of Xen clusters in the alpha cages of zeolite AgA. Journal of Chemical Physics, 1997, 107, 4373-4383.	1.2	16
115	Xe Chemical Shift Tensor in Silicalite and SSZ-24. Journal of the American Chemical Society, 2004, 126, 10450-10456.	6.6	16
116	Exploring gas permeability of lipid membranes using coarse-grained molecular dynamics. Molecular Simulation, 2009, 35, 953-961.	0.9	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 19F shielding in CF2=CFX and CF2=CH2. Journal of Chemical Physics, 1985, 83, 5425-5433.	1.2	15
119	Gasâ€toâ€liquid shifts in NMR and the validity of the second virial coefficient of chemical shielding. Journal of Chemical Physics, 1979, 70, 5916-5917.	1.2	14
120	The role of polarization of Xe by di- and monovalent cations in 129Xe NMR studies in zeolite A. Solid State Nuclear Magnetic Resonance, 1997, 9, 277-301.	1.5	14
121	Quantum-mechanical treatment of the electronic structure and geometry of hydrogen cyanide dimer. Journal of Theoretical Biology, 1972, 35, 247-257.	0.8	13
122	Variation of chemical shielding with intermolecular interactions and rovibrational motion. III. 31P nucleus in PH3. Journal of Chemical Physics, 1978, 68, 2868.	1.2	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.	1.9	13
124	Cross sections for the anisotropic interaction of NNO with various molecules. Journal of Chemical Physics, 1988, 89, 5642-5649.	1.2	13
125	Rotational behaviour of PEGylated gold nanorods in a lipid bilayer system. Molecular Physics, 2017, 115, 1122-1143.	0.8	13
126	Isotope effects in 31P 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 19F chemical shielding in CH3F. Journal of Chemical Physics, 1978, 69, 1655-1660.	1.2	12
128	Temperature dependence of the chemical shielding of 19F nuclei in isolated CF3H, CF3Cl, CF3Br, and CF3CF3 molecules. Journal of Chemical Physics, 1978, 69, 1318.	1.2	12
129	The mean bond displacements in O=CF2 and their effect on 19F nuclear magnetic shielding. Journal of Chemical Physics, 1984, 81, 4915-4921.	1.2	12
130	Nuclear spin relaxation studies of the spinâ€rotation interaction of 13C in CO in various buffer gases. Journal of Chemical Physics, 1986, 85, 697-700.	1.2	12
131	Molecular Dynamics Simulations of Xe Chemical Shifts and Solubility in n-Alkanes. Journal of Physical Chemistry C, 2007, 111, 15771-15783.	1.5	12
132	Measuring chirality in NMR in the presence of a static electric field. Journal of Chemical Physics, 2008, 128, 154502.	1.2	12
133	Diffusion of gases across lipid membranes with OmpA channel: a molecular dynamics study. Molecular Physics, 2010, 108, 1569-1581.	0.8	12
134	Variation of nuclear magnetic shielding with intermolecular interactions and rovibrational motion. IX. 19F in F2C=CH2 and F2C=CF2. Journal of Chemical Physics, 1984, 81, 2571-2573.	1.2	11
135	Variation of nuclear magnetic shielding with intermolecular interactions and rovibrational motion. VIII. 19F in CF3X. Journal of Chemical Physics, 1984, 81, 1198-1202.	1.2	11
136	Quadrupolar spin relaxation due to electric field gradients induced by vibrations and collisions. Molecular Physics, 1986, 57, 553-571.	0.8	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.	1.2	11
138	Vibrational analysis and mean bond displacements in M(XY)6 complexes. Journal of the American Chemical Society, 1987, 109, 2586-2588.	6.6	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.	0.9	10
140	The Parameters of NMR Spectroscopy. , 1987, , 3-50.		10
141	Relaxation cross sections for the rotational angular momentum vector in CF4. Journal of Chemical Physics, 1988, 89, 866-870.	1.2	9
142	Nuclear magnetic shielding and chirality. III. The single electron on a helix model. Journal of Chemical Physics, 2003, 119, 2694-2701.	1.2	8
143	Prediction of Henry's constants of xenon in cyclo-alkanes from molecular dynamics simulations. Fluid Phase Equilibria, 2008, 269, 73-79.	1.4	8
144	Molecular dynamics simulations of enantiomeric separations as an interfacial process in <scp>HPLC</scp>. AICHE Journal, 2021, 67, e17143.	1.8	8

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145	Rovibrational Averaging of Molecular Electronic Properties. , 1991, , 457-519.		8
146	Effects of vibrational anharmonicity on19F nuclear resonance in SF6. Molecular Physics, 1980, 40, 999-1003.	0.8	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.	1.2	7
148	Xe nuclear magnetic resonance line shapes in channels decorated with paramagnetic centers. Journal of Chemical Physics, 2006, 125, 114708.	1.2	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.	1.0	7
150	Fluorine. , 1987, , 437-446.		7
151	Theoretical and physical aspects of nuclear shielding. Nuclear Magnetic Resonance, 0, , 42-76.	0.1	7
152	Variation of chemical shielding with intermolecular interactions and rovibrational motion. VI. 19F in SF4 and COF2. Journal of Chemical Physics, 1981, 74, 1613-1617.	1.2	6
153	19F nuclear spin relaxation by intermolecular magnetic dipole coupling. CF4and SiF4in oxygen gas. Journal of Chemical Physics, 1991, 94, 172-178.	1.2	6
154	On using the NMR chemical shift to assess polarâ€“nonpolar cross-intermolecular interactions. Chemical Physics Letters, 2003, 380, 556-562.	1.2	6
155	Intermolecular hyperfine tensor for Xe@O2. Density and temperature dependence of Xe chemical shifts in oxygen gas. Molecular Physics, 2006, 104, 1217-1225.	0.8	6
156	Theoretical and physical aspects of nuclear shielding. Nuclear Magnetic Resonance, 2015, , 46-75.	0.1	6
157	Effect of centrifugal distortion and anharmonic vibration on the chemical shielding of 31P in PH3 and PD3. Journal of Chemical Physics, 1978, 69, 615-621.	1.2	5
158	Variation of nuclear magnetic shielding of 19F 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 SF6 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.	1.1	5
162	Quadrupolar spin relaxation of 14N in NNO in collisions with various molecules. Journal of Chemical Physics, 1998, 109, 10227-10237.	1.2	5

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163	Molecular dynamics simulations of chiral recognition of drugs by amylose polymers coated on amorphous silica. Molecular Physics, 2021, 119, .	0.8	5
164	Theoretical and physical aspects of nuclear shielding. Nuclear Magnetic Resonance, 0, , 1-17.	0.1	5
165	The temperature dependence of the19F resonance in isolated F2C=CFX molecules. Journal of Chemical Physics, 1985, 83, 5420-5424.	1.2	4
166	Is there a spatial correlation in the distribution of adsorbed atoms in the cages of a zeolite?. Molecular Physics, 2004, 102, 723-727.	0.8	4
167	Molecular reorientation of CD4 in gas-phase mixtures. Magnetic Resonance in Chemistry, 2006, 44, 241-248.	1.1	4
168	Molecular Dynamics Studies of Nanoparticle Transport Through Model Lipid Membranes. , 2019, , 109-165.		4
169	Novel methods to characterise spatial distribution and enantiomeric composition of usnic acids in four Icelandic lichens. Phytochemistry, 2022, 200, 113210.	1.4	4
170	Molecular reorientation of nearly classical spherical tops: selenium hexafluoride and tellurium hexafluoride. The Journal of Physical Chemistry, 1991, 95, 2982-2988.	2.9	3
171	Theoretical and physical aspects of nuclear shielding. Nuclear Magnetic Resonance, 2012, , 38-55.	0.1	3
172	Computer-enriched modules for introductory chemistry. Journal of Chemical Education, 1977, 54, 238.	1.1	2
173	A classical dynamics study of the anisotropic interactions in NNOâ€“Ar and NNOâ€“Kr systems: Comparison with transport and relaxation data. Journal of Chemical Physics, 1998, 109, 10238-10243.	1.2	2
174	Theoretical and physical aspects of nuclear shielding. Nuclear Magnetic Resonance, 0, , 51-67.	0.1	2
175	Molecular-Level â€œObservationsâ€•of the Behavior of Gold Nanoparticles in Aqueous Solution and Interacting with a Lipid Bilayer Membrane. Methods in Molecular Biology, 2019, 2000, 303-359.	0.4	2
176	Interfacial Thermal Conductivity and Its Anisotropy. Processes, 2020, 8, 27.	1.3	2
177	Theoretical and physical aspects of nuclear shielding. Nuclear Magnetic Resonance, 0, , 1-30.	0.1	2
178	Using Molecular Simulations to Facilitate Design and Operation of Membrane-Based and Chiral Separation Processes. Industrial & Engineering Chemistry Research, 2022, 61, 15554-15566.	1.8	2
179	Response to â€˜â€˜Comment on â€˜14N spin relaxation studies of N2in buffer gases. Cross sections for molecular reorientation and rotational energy transferâ€™â€‰â€™ [J. Chem. Phys.100, 1775 (1994)]. Journal of Chemical Physics, 1994, 100, 1777-1778.		1
180	Application of Nuclear Shielding Surfaces to the Fundamental Understanding of Adsorption and Diffusion in Microporous Solids. ACS Symposium Series, 1999, , 335-348.	0.5	1

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181	Recent Advances in Nuclear Magnetic Shielding Theory and Computational Methods. ACS Symposium Series, 1999, , 1-23.	0.5	1
182	Theoretical and physical aspects of nuclear shielding. Nuclear Magnetic Resonance, 2011, , 37-54.	0.1	1
183	Understanding Separation Mechanisms of Monoatomic Gases, Such as Kr and Xe, via DD3R Zeolite Membrane Using Molecular Dynamics. Thermo, 2022, 2, 56-73.	0.6	1
184	Reply to a comment on: Angular momentum relaxation in binary collisions. Comparison of cross sections. Journal of Chemical Physics, 1991, 94, 7565-7565.	1.2	0
185	Chapter 2. Theoretical and physical aspects of nuclear shielding. Nuclear Magnetic Resonance, 2014, , 49-80.	0.1	0