Roy E Bruns

List of Publications by Year
in descending order

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265	6,594	159585	88630
papers	citations	30 h-index	70 g-index

275	275	275	6526
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Box-Behnken design: An alternative for the optimization of analytical methods. Analytica Chimica Acta, 2007, 597, 179-186.	5.4	2,226
2	Statistical designs and response surface techniques for the optimization of chromatographic systems. Journal of Chromatography A, 2007, 1158, 2-14.	3.7	493
3	The removal of the indigo carmine dye from aqueous solutions using cross-linked chitosanâ€"Evaluation of adsorption thermodynamics using a full factorial design. Journal of Hazardous Materials, 2008, 153, 566-574.	12.4	97
4	An Atomic Chargeâ^'Charge Fluxâ^'Dipole Flux Atom-in-Molecule Decomposition for Molecular Dipole-Moment Derivatives and Infrared Fundamental Intensities. Journal of Physical Chemistry A, 2005, 109, 2680-2688.	2.5	80
5	Flow injection systems with inductively-coupled argon plasma atomic emission spectrometry. Analytica Chimica Acta, 1981, 130, 243-255.	5.4	76
6	Simulation of an industrial wastewater treatment plant using artificial neural networks and principal components analysis. Brazilian Journal of Chemical Engineering, 2002, 19, 365-370.	1.3	68
7	Statistical design-principal component analysis optimization of a multiple response procedure using cloud point extraction and simultaneous determination of metals by ICP OES. Analytica Chimica Acta, 2006, 580, 251-257.	5.4	66
8	Title is missing!. Biotechnology Letters, 2001, 23, 1963-1969.	2.2	56
9	Emission of polycyclic aromatic hydrocarbons from gasohol and ethanol vehicles. Atmospheric Environment, 2009, 43, 648-654.	4.1	54
10	Calculated Dipoleâ€Moment Functions and the Infrared Intensities of HCN and N2O. Journal of Chemical Physics, 1970, 53, 1413-1417.	3.0	53
11	Use of multivariate statistical techniques to optimize the simultaneous separation of 13 phenolic compounds from extra-virgin olive oil by capillary electrophoresis. Talanta, 2011, 83, 1181-1187.	5.5	52
12	Optimisation of a CE method for caffeine analysis in decaffeinated coffee. Food Chemistry, 2010, 120, 1155-1161.	8.2	47
13	The removal of Cu(II) and Co(II) from aqueous solutions using cross-linked chitosanâ€"Evaluation by the factorial design methodology. Journal of Hazardous Materials, 2007, 143, 8-16.	12.4	45
14	Simultaneous determination of first-line anti-tuberculosis drugs by capillary zone electrophoresis using direct UV detection. Talanta, 2010, 82, 333-339.	5.5	45
15	Experimental mixture design solvent effects on pigment extraction and antioxidant activity from Coffea arabica L. leaves. Microchemical Journal, 2019, 146, 713-721.	4.5	45
16	Atomic Mean Dipole Moment Derivatives and GAPT Charges. Journal of Physical Chemistry A, 2000, 104, 5320-5327.	2.5	40
17	Application of steady-state and dynamic modeling for the prediction of the BOD of an aerated lagoon at a pulp and paper millPart II. Nonlinear approaches. Chemical Engineering Journal, 2004, 105, 61-69.	12.7	40
18	Principal component analysis and hierarchical cluster analysis for homogeneity evaluation during the preparation of a wheat flour laboratory reference material for inorganic analysis. Microchemical Journal, 2010, 95, 222-226.	4.5	40

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19	How Accessible Is Atomic Charge Information from Infrared Intensities? A QTAIM/CCFDF Interpretation. Journal of Physical Chemistry A, 2012, 116, 8238-8249.	2.5	40
20	Controlled Release of 2,4-D from Granule Matrix Formulations Based on Six Lignins. Journal of Agricultural and Food Chemistry, 1997, 45, 1001-1005.	5.2	38
21	Core Electron Energies, Infrared Intensities, and Atomic Charges. Journal of the American Chemical Society, 1997, 119, 4224-4231.	13.7	38
22	Factorial design of electrolyte systems for the separation of fatty acids by capillary electrophoresis. Journal of Chromatography A, 2001, 924, 533-539.	3.7	38
23	Mineral composition of wheat flour consumed in Brazilian cities. Journal of the Brazilian Chemical Society, 2008, 19, 935-942.	0.6	36
24	CNDO Calculation of Dipole Moment Derivatives and Infrared Intensities of C6H6 and C6F6. Journal of Chemical Physics, 1972, 57, 324-331.	3.0	35
25	Dioxins and furans in the atmosphere of SÃ£o Paulo City, Brazil. Chemosphere, 2005, 58, 1391-1398.	8.2	35
26	Water-Soluble Ions and Trace Metals in Airborne Particles Over Urban Areas of the State of SÃ£o Paulo, Brazil: Influences of Local Sources and Long Range Transport. Water, Air, and Soil Pollution, 2007, 186, 63-73.	2.4	35
27	Calculation of the Vibrational Intensities of F2CO. Journal of Chemical Physics, 1969, 50, 3811-3812.	3.0	31
28	A fast procedure for standard additions in flow injection analysis. Analytica Chimica Acta, 1985, 171, 337-343.	5.4	31
29	A Simple Potential Model Criterion for the Quality of Atomic Charges. Journal of Physical Chemistry A, 1999, 103, 4918-4924.	2.5	31
30	Experimental determination of relative signs of dipole moment derivatives: HCN and DCN. Journal of Chemical Physics, 1978, 68, 847-851.	3.0	30
31	32 Factorial design and response surface analysis optimization of N-carboxybutylchitosan synthesis. Carbohydrate Polymers, 2005, 59, 37-42.	10.2	30
32	Mixtureâ€“mixture design for the fingerprint optimization of chromatographic mobile phases and extraction solutions for Camellia sinensis. Analytica Chimica Acta, 2007, 595, 28-37.	5.4	30
33	Vibrational Intensities in F2CO: Some Corrections. Journal of Chemical Physics, 1971, 55, 2890-2894.	3.0	29
34	CNDO calculation of dipole moment derivatives and infrared intensities of formaldehyde. Journal of Chemical Physics, 1973, 58, 2585-2592.	3.0	29
35	SENSORY EVALUATION OF ORANGE JUICE CONCENTRATE AS AFFECTED BY IRRADIATION AND STORAGE. Journal of Food Processing and Preservation, 1997, 21, 179-191.	2.0	29
36	Hidrocarbonetos policÃclicos aromÃ¡ticos como traÃ§adores da queima de cana-de-aÃ§Ãºcar: uma abordagem estatÃstica. Quimica Nova, 2007, 30, 577-581.	0.3	29

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37	The polar tensors, effective charges, and infrared intensities of X2CY molecules. Journal of Chemical Physics, 1975, 62, 3235-3239.	3.0	28
38	New Factorial Designs to Evaluate Chemisorption of Divalent Metals on Aminated Silicas. Journal of Colloid and Interface Science, 2001, 241, 45-51.	9.4	28
39	Multivariate optimisation of ICP OES instrumental parameters for Pb/Ba/Sb measurement in gunshot residues. Microchemical Journal, 2015, 120, 58-63.	4.5	28
40	Infrared gas phase intensity measurements, polar tensors, and effective charges of cisâ€difluoroethylene and its deuterated modifications. Journal of Chemical Physics, 1983, 78, 7029-7037.	3.0	27
41	Characterization of monofloral honeys by ash contents through a hierarchical design. Journal of Food Composition and Analysis, 2004, 17, 737-747.	3.9	27
42	Doehlert design-desirability function multi-criteria optimal separation of 17 phenolic compounds from extra-virgin olive oil by capillary zone electrophoresis. Food Chemistry, 2014, 146, 558-568.	8.2	27
43	QTAIM Chargeâ^'Charge Fluxâ^'Dipole Flux Models for the Infrared Fundamental Intensities of the Fluorochloromethanes. Journal of Physical Chemistry A, 2006, 110, 4839-4845.	2.5	26
44	Statistical mixture design â€" Principal component determination of synergic solvent interactions for natural product extractions. Chemometrics and Intelligent Laboratory Systems, 2010, 103, 1-7.	3.5	26
45	Principal component analysis of dipole moment derivative signs of chloroform. Journal of Computational Chemistry, 1991, 12, 885-890.	3.3	25
46	A chemometric analysis ofab initio vibrational frequencies and infrared intensities of methyl fluoride. Journal of Computational Chemistry, 1996, 17, 167-177.	3.3	25
47	Methylene blue immobilized on cellulose surfaces modified with titanium dioxide and titanium phosphate: factorial design optimization of redox properties. Journal of Electroanalytical Chemistry, 2002, 531, 141-146.	3.8	25
48	Evaluation of the salt accumulation process during inundation in water resource of Contas river basin (Bahiaâ€"Brazil) applying principal component analysis. Water Research, 2004, 38, 1579-1585.	11.3	25
49	Determination of Cd, Cu, and Pb after Cloud Point Extraction using Multielemental Sequential Determination by Thermospray Flame Furnace Atomic Absorption Spectrometry (TSâ€FFâ€AAS). Separation Science and Technology, 2008, 43, 815-827.	2.5	25
50	Statistical mixture design investigation of fractionated and total extracts from Erythrina speciosa Andrews leaves. Journal of Separation Science, 2009, 32, 644-652.	2.5	25
51	Combined columnâ€"mobile phase mixture statistical design optimization of high-performance liquid chromatographic analysis of multicomponent systems. Journal of Chromatography A, 2009, 1216, 1439-1449.	3.7	25
52	A fractional factorial design applied to organofunctionalized silicas for adsorption optimization. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 1996, 117, 7-13.	4.7	24
53	Infrared gas phase intensity measurements, polar tensors, and effective charges of vinylidene fluoride and its deuterated modifications. Journal of Chemical Physics, 1982, 77, 1099-1106.	3.0	23
54	Application of steady-state and dynamic modeling for the prediction of the BOD of an aerated lagoon at a pulp and paper mill. Chemical Engineering Journal, 2004, 104, 73-81.	12.7	23

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55	Automatic on-line pre-concentration system using a knotted reactor for the FAAS determination of lead in drinking water. Journal of Hazardous Materials, 2007, 141, 540-545.	12.4	23
56	Determination of Flavanones in Orange Juices Obtained from Different Sources by HPLC/DAD. Journal of Analytical Methods in Chemistry, 2014, 2014, 1-5.	1.6	23
57	25 anos de quimiometria no Brasil. Quimica Nova, 2006, 29, 1401-1406.	0.3	22
58	Quantum Theory of Atoms in Molecules Chargeâ^'Charge Fluxâ^'Dipole Flux Models for the Infrared Intensities of X₂CY (X = H, F, Cl; Y = O, S) Molecules. Journal of Physical Chemistry A, 2007, 111, 7870-7875.	2.5	22
59	ChelpG and QTAIM atomic charge and dipole models for the infrared fundamental intensities of the fluorochloromethanes. Theoretical Chemistry Accounts, 2008, 121, 173-179.	1.4	22
60	CNDO Calculation of Dipoleâ€Moment Derivatives and Infrared Intensities of BF3. Journal of Chemical Physics, 1971, 55, 5401-5404.	3.0	21
61	Mean dipole moment derivatives, atomic anisotropies, and effective charges of diatomic hydrides. Journal of Chemical Physics, 1978, 68, 880-885.	3.0	21
62	Application of the split-plot experimental design for the optimization of a catalytic procedure for the determination of Cr(VI). Analytica Chimica Acta, 1998, 369, 269-279.	5.4	21
63	Title is missing!. World Journal of Microbiology and Biotechnology, 1998, 14, 487-490.	3.6	21
64	Electrospray ionization mass spectrometry fingerprinting of perfumes: rapid classification and counterfeit detection. Rapid Communications in Mass Spectrometry, 2006, 20, 3654-3658.	1.5	21
65	Vibrational intensities of F2CO, Cl2CO, and Br2CO. Journal of Chemical Physics, 1973, 58, 1849-1854.	3.0	20
66	Catalytic determination of molybdenum (VI) in plants using mono-segmented continuous-flow analysis and spectrophotometric detection. Analyst, The, 1993, 118, 213.	3.5	20
67	Effects of wave function modifications on calculated Cî—¸H vibrational frequencies and infrared intensities of the dihaloethylenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 733-747.	3.9	20
68	Infrared Vibrational Intensities, Polar Tensors, and Core Electron Energies of the Group IV Hydrides and the Fluorosilanes. Journal of Physical Chemistry A, 1998, 102, 4615-4622.	2.5	20
69	A chargeâ€“charge fluxâ€“dipole flux decomposition of the dipole moment derivatives and infrared intensities of the AB3 (A=N, P; B=H, F) molecules. Chemical Physics, 2005, 317, 35-42.	1.9	20
70	Optimization of an electrolyte system for analysis of ethambutol in pharmaceutical formulations by capillary zone electrophoresis using complexation with copper(II). Journal of Chromatography A, 2008, 1202, 224-228.	3.7	20
71	STATISTICAL DESIGN OF EXPERIMENTS FOR OPTIMIZATION OF BATCH ADSORPTION CONDITIONS FOR REMOVAL OF REACTIVE RED 194 TEXTILE DYE FROM AQUEOUS EFFLUENTS. Chemical Engineering Communications, 2010, 197, 775-790.	2.6	20
72	Vibrational intensities of F2CS and Cl2CS. Journal of Chemical Physics, 1973, 58, 1855-1860.	3.0	19

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73	Comparison of Methods for Determining Moisture Content of Citrus and Eucalyptus Brazilian Honeys by Refractometry. Journal of Food Composition and Analysis, 2001, 14, 101-109.	3.9	19
74	Factorial design optimization of solid phase microextraction conditons for gas chromatographyâ€“mass spectrometry (GCâ€“MS) analysis of linear alkylbenzenes (LABs) in detergents. Analytica Chimica Acta, 2006, 562, 152-157.	5.4	19
75	Statistical mixture designâ€”Varimax factor optimization for selective compound extraction from plant material. Analytica Chimica Acta, 2008, 613, 48-55.	5.4	19
76	Sequential mixture design optimization for divergent metabolite analysis: Enriched carbon dioxide effects on Coffea arabica L. leaves and buds. Talanta, 2019, 191, 382-389.	5.5	19
77	The carbonyl vibration in Î±-Group IV metal ketones. Journal of Organometallic Chemistry, 1973, 56, 131-140.	1.8	18
78	Factorial design optimization of redox properties of methylene blue adsorbed on a modified silica gel surface. Journal of Electroanalytical Chemistry, 1997, 433, 73-76.	3.8	18
79	Optimization of thermogravimetric analysis of ash content in honey. Journal of the Brazilian Chemical Society, 2004, 15, 797-802.	0.6	18
80	ImplementaÃ§Ã£o computacional do modelo carga-fluxo de carga-fluxo de dipolo para cÃ¡lculo e interpretaÃ§Ã£o das intensidades do espectro infravermelho. Quimica Nova, 2008, 31, 1750-1754.	0.3	18
81	Development of a new topological index for the prediction of normal boiling point temperatures of hydrocarbons: The Fi index. Journal of Molecular Liquids, 2012, 165, 125-132.	4.9	18
82	Experimental designs characterizing seasonal variations and solvent effects on the quantities of coumarin and related metabolites from Mikania laevigata. Analytica Chimica Acta, 2014, 821, 89-96.	5.4	18
83	Infrared gas phase intensity measurements. Polar tensors and effective charges of cisâ€dichloroethyleneâ€d0 and d2. Journal of Chemical Physics, 1983, 79, 19-25.	3.0	17
84	Flow injection calibration of inductively coupled plasma atomic emission spectrometry using the generalised standard additions method. Journal of Analytical Atomic Spectrometry, 1988, 3, 673-678.	3.0	17
85	A multivariate statistical analysis of the composition of rainwater near CubatÃ£o, SP, Brazil. Environmental Pollution, 1993, 79, 225-233.	7.5	17
86	Principal component analysis of the cis- and trans-difluoroethylene polar tensors. The Journal of Physical Chemistry, 1993, 97, 6161-6166.	2.9	17
87	QTAIM Chargeâ”Charge Fluxâ”Dipole Flux Models for the Infrared Fundamental Intensities of Difluoro- and Dichloroethylenes. Journal of Physical Chemistry A, 2007, 111, 515-520.	2.5	17
88	Statistical mixture design development of digestion methods for Oyster tissue using inductively coupled plasma optical emission spectrometry for the determination of metallic ions. Talanta, 2009, 80, 559-564.	5.5	17
89	Chemometrics optimization of carbohydrate separations in six food matrices by micellar electrokinetic chromatography with anionic surfactant. Talanta, 2011, 85, 237-244.	5.5	17
90	Characteristic infrared intensities of carbonyl stretching vibrations. Physical Chemistry Chemical Physics, 2016, 18, 17575-17585.	2.8	17

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91	An electronegativity model for vibrational intensities of substituted methanes. Journal of Chemical Physics, 1988, 89, 1887-1891.	3.0	16
92	Atomic charge transfer-counter polarization effects determine infrared CH intensities of hydrocarbons: a quantum theory of atoms in molecules model. Physical Chemistry Chemical Physics, 2014, 16, 23224-23232.	2.8	16
93	Dynamic atomic contributions to infrared intensities of fundamental bands. Physical Chemistry Chemical Physics, 2015, 17, 30378-30388.	2.8	16
94	The polar tensors, atomic effective charges, and infrared vibrational intensities of C6H6, C6D6, and C6F6. Journal of Chemical Physics, 1978, 68, 5451-5458.	3.0	15
95	Electronegativity Models for the Infrared Vibrational Intensities of the Halomethanes. Journal of the American Chemical Society, 1995, 117, 4144-4150.	13.7	15
96	PARAFAC HPLC-DAD metabolomic fingerprint investigation of reference and crossed coffees. Food Research International, 2018, 113, 9-17.	6.2	15
97	Are â€œGAPT Chargesâ€•Really Just Charges?. Journal of Chemical Information and Modeling, 2021, 61, 3881-3890.	5.4	15
98	G sum rule applications for the vibrational intensities of the hydrocarbons. Journal of Chemical Physics, 1979, 71, 5042.	3.0	14
99	Principal component analysis of the polar tensors of difluoromethane and difluoromethane-d2. The Journal of Physical Chemistry, 1991, 95, 9716-9720.	2.9	14
100	Multi-component principal component regression and partial least-squares analyses of overlapped chromatographic peaks. Journal of Chromatography A, 1991, 539, 123-132.	3.7	14
101	A principal component analysis of the methyl fluoride polar tensors. Computational and Theoretical Chemistry, 1993, 282, 81-89.	1.5	14
102	Some New Data for Metal Desorption on Inorganicâ€“Organic Hybrid Materials. Journal of Colloid and Interface Science, 2000, 227, 66-70.	9.4	14
103	Title is missing!. Journal of Applied Electrochemistry, 2003, 33, 1069-1075.	2.9	14
104	Factorial design effects of plant density, pattern and light availability on the caffeine, chlorogenic acids, lipids, reducing sugars and ash contents of Coffea arabica L. beans and leaves. Analytical Methods, 2017, 9, 3612-3618.	2.7	14
105	Seasonal changes and solvent effects on fractionated functional food component yields from Mikania laevigata leaves. Food Chemistry, 2019, 273, 151-158.	8.2	14
106	Factorial design fingerprint discrimination of Coffea arabica beans under elevated carbon dioxide and limited water conditions. Talanta, 2020, 209, 120591.	5.5	14
107	Spectroscopic and Chromatographic Fingerprints for Discrimination of Specialty and Traditional Coffees by Integrated Chemometric Methods. Food Analytical Methods, 2020, 13, 2204-2212.	2.6	14
108	Transferability of the cis- and trans-difluoroethylene polar tensors. The Journal of Physical Chemistry, 1985, 89, 4979-4983.	2.9	13

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109	Effects of wave function modifications on calculated Cî—¸F and Cî—¸Cl vibrational frequencies and infrared intensities of the dihaloethylenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 1563-1579.	3.9	13
110	Study of the reaction conditions for the hydrodechlorination of pentachlorophenol on palladium catalysts. Chemical Engineering Journal, 2007, 131, 59-64.	12.7	13
111	Principal component and Tucker3 analyses of high performance liquid chromatography with diode-array detection fingerprints of crude extracts of Erythrina speciosa Andrews leaves. Analytica Chimica Acta, 2012, 736, 36-44.	5.4	13
112	An atom in molecules study of infrared intensity enhancements in fundamental donor stretching bands in hydrogen bond formation. Physical Chemistry Chemical Physics, 2014, 16, 24920-24928.	2.8	13
113	Chemometric Analysis of 1H NMR Fingerprints of Coffea arabica Green Bean Extracts Cultivated under Different Planting Densities. Food Analytical Methods, 2018, 11, 1906-1914.	2.6	13
114	Mixture Design PARAFAC HPLC-DAD Metabolomic Fingerprints of Fractionated Organic and Basic Extracts from Erythrina speciosa Andrews Leaves. Chromatographia, 2018, 81, 1189-1200.	1.3	13
115	Potential biomonitoring of atmospheric carbon dioxide in Coffea arabica leaves using near-infrared spectroscopy and partial least squares discriminant analysis. Environmental Science and Pollution Research, 2019, 26, 30356-30364.	5.3	13
116	Dipole moment derivatives, polar tensors, and effective charges of ammonia and phosphine. The Journal of Physical Chemistry, 1976, 80, 2768-2770.	2.9	12
117	Similarity transference of molecular parameters. II. The bond distances, force constants and polar tensors of HC3N and HC5N. Journal of Chemical Physics, 1989, 90, 6933-6939.	3.0	12
118	Atomic Mean Dipole Moment Derivative and Anisotropic Contributions to Molecular Infrared Intensity Sums. Journal of Physical Chemistry A, 2004, 108, 6788-6796.	2.5	12
119	Statistical mixture design â€“ principal component optimization for selective compound extraction from plant material. Journal of Separation Science, 2007, 30, 3302-3310.	2.5	12
120	Multivariate optimization and validation of an analytical method for the determination of cadmium in wines employing ET AAS. Journal of the Brazilian Chemical Society, 2009, 20, 788-794.	0.6	12
121	Infrared Intensification and Hydrogen Bond Stabilization: Beyond Point Charges. Journal of Physical Chemistry A, 2019, 123, 6482-6490.	2.5	12
122	Environmental stress evaluation of Coffea arabica L. leaves from spectrophotometric fingerprints by PCA and OSCâ€“PLSâ€“DA. Arabian Journal of Chemistry, 2019, 12, 4251-4257.	4.9	12
123	The main effects of elevated CO2 and soil-water deficiency on 1H NMR-based metabolic fingerprints of Coffea arabica beans by factorial and mixture design. Science of the Total Environment, 2020, 749, 142350.	8.0	12
124	FT-IR biomarkers of sexual dimorphism in yerba-mate plants: Seasonal and light accessibility effects. Microchemical Journal, 2020, 158, 105329.	4.5	12
125	A localized molecular orbital interpretation of the dipole moment derivatives of ammonia. A reexamination of the bond moment model description of infrared intensities. Journal of the American Chemical Society, 1976, 98, 3432-3435.	13.7	11
126	The theoretical calculation of polar tensors and dipole moment derivatives: BF3 and Bcl3. Journal of Chemical Physics, 1976, 64, 3053-3056.	3.0	11

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127	Mean dipole moment derivatives and anisotropies of X2CY molecules. Journal of Chemical Physics, 1976, 64, 3084-3085.	3.0	11
128	Study of the Mo(VI) catalytic response in the oxidation of iodide by hydrogen peroxide using a monosegmented continuous-flow system. Analytica Chimica Acta, 1991, 255, 149-155.	5.4	11
129	Split-plot design optimization for trace determination of lead by anodic stripping voltammetry in a homogeneous ternary solvent system. Chemometrics and Intelligent Laboratory Systems, 2004, 70, 113-121.	3.5	11
130	Characteristic Substituent-Shift Models for Carbon 1s Ionization Energies and Mean Dipole-Moment Derivatives. Journal of Physical Chemistry A, 2004, 108, 866-873.	2.5	11
131	Factorial design to optimize microwave-assisted synthesis of FDU-1 silica with a new triblock copolymer. Microporous and Mesoporous Materials, 2010, 133, 1-9.	4.4	11
132	Mixture designs for exploring class diversity and metabolite fingerprinting: An efficient column chromatographic strategy. Analytica Chimica Acta, 2011, 702, 288-294.	5.4	11
133	Quantum theory of atoms in molecules/charge-charge flux-dipole flux models for fundamental vibrational intensity changes on H-bond formation of water and hydrogen fluoride. Journal of Chemical Physics, 2014, 140, 084306.	3.0	11
134	Variation of the Distribution of Atmospheric n-Alkanes Emitted by Different Fuelsâ€™ Combustion. Atmosphere, 2020, 11, 643.	2.3	11
135	Acidities and spectral properties of .alpha.-silyl and .alpha.-germyl carboxylic acids and their carboxylates. Journal of the American Chemical Society, 1972, 94, 9087-9092.	13.7	10
136	Polymer-polymer miscibility evaluation by acoustic emission. Die Makromolekulare Chemie Rapid Communications, 1992, 13, 45-53.	1.1	10
137	Optimization through Factorial Planning of the Use of Ethanol : Water as a Mobile Phase for Reversed Phase HPLC. Journal of High Resolution Chromatography, 1999, 22, 52-54.	1.4	10
138	UV-Vis spectral fingerprinting and chemometric method applied to the evaluation of Camellia sinensis leaves from different harvests. Analytical Methods, 2016, 8, 7537-7544.	2.7	10
139	Effect of selenium treated broccoli on herbivory and oviposition preferences of Delia radicum and Phyllotreta spp.. Scientia Horticulturae, 2017, 225, 445-453.	3.6	10
140	Irrigated and CO2 level effects on metabolism in Coffea arabica beans from mixture design â€“ near infrared fingerprints. Microchemical Journal, 2020, 152, 104276.	4.5	10
141	F and G intensity sum rule applications: the CHxD4âˆ’x molecules. Journal of Chemical Physics, 1978, 69, 4147-4148.	3.0	9
142	Gâ€intensity sum rule applications: XY3 molecules. Journal of Chemical Physics, 1978, 68, 5448-5450.	3.0	9
143	Similarity transference of molecular parameters. I. The atomic polar tensors of cyanoacetylene. Journal of Chemical Physics, 1986, 85, 4515-4523.	3.0	9
144	An application of chemometric techniques to the study of ab initio rotational constants of linear molecules. Chemometrics and Intelligent Laboratory Systems, 1998, 44, 187-195.	3.5	9

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145	Optimization of mobile phase for separation of carbohydrates in honey by high performance liquid chromatography using a mixture design. Journal of the Brazilian Chemical Society, 2006, 17, 588-593.	0.6	9
146	EstatÃstica aplicada Ã quÃmica: dez dÃºvidas comuns. Quimica Nova, 2011, 34, 888-892.	0.3	9
147	Mixture Design Optimization of an Analytical Procedure for Iron Extraction and Determination From Cassava Leaves by Slurry Sampling Flame Atomic Absorption Spectrometry. Spectroscopy Letters, 2011, 44, 388-392.	1.0	9
148	Quantum Theory of Atoms in Molecules/Chargeâ€“Charge Fluxâ€“Dipole Flux interpretation of fundamental vibrational intensity enhancements on H-bond formation of water trimer. Chemical Physics Letters, 2014, 610-611, 14-18.	2.6	9
149	OtimizaÃ§Ã£o via metodologia de superfÃcie de respostas dos parÃ¢metros tecnolÃ³gicos para produÃ§Ã£o de fruta estruturada e desidratada a partir de polpa concentrada de mamÃ£o. Food Science and Technology, 2005, 25, 158-164.	1.7	9
150	Regularities in calculated dipole moment derivatives of first row diatomic hydrides. Journal of Chemical Physics, 1974, 61, 1779-1781.	3.0	8
151	Polar tensors and effective charges of carbonic dibromide. The Journal of Physical Chemistry, 1975, 79, 1880-1882.	2.9	8
152	Donorâ€”acceptor interactions of substituted benzenes with molecular chlorine and carbon disulfide. Journal of Molecular Structure, 1975, 29, 211-223.	3.6	8
153	On the structure of the benzene-chlorine complex: a CNDO study. Journal of Molecular Structure, 1977, 36, 121-126.	3.6	8
154	F and G sum rules as error indicators of experimental vibrational intensity data: The CHxD3â^'xBr molecules. Journal of Chemical Physics, 1978, 69, 3374-3378.	3.0	8
155	Principal component analyses of the methyl chloride, bromide, and iodide polar tensors. The Journal of Physical Chemistry, 1993, 97, 4354-4359.	2.9	8
156	Multivariate statistical investigation of the effects of wave function modifications on the calculated vibrational frequencies and infrared intensities of CH2F2. Computational and Theoretical Chemistry, 1997, 394, 197-208.	1.5	8
157	Vibrational intensities and directions of the dipolar derivatives of the trans- C2H2X2 (X F or Cl). Journal of Molecular Structure, 1999, 482-483, 585-589.	3.6	8
158	Factorial design analysis of the catalytic activity of di-imine copper(II) complexes in the decomposition of hydrogen peroxide. International Journal of Chemical Kinetics, 2001, 33, 472-479.	1.6	8
159	The infrared vibrational intensities and polar tensors of HFCO and DFCO. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 2947-2952.	3.9	8
160	Full factorial design applied to intercalation of amines in lamellar titanium phenylphosphonate and titanium phenylarsonate. Journal of Solid State Chemistry, 2004, 177, 675-680.	2.9	8
161	Technological aspects for restructuring concentrated pineapple pulp. LWT - Food Science and Technology, 2007, 40, 759-765.	5.2	8
162	Unreplicated split-plot mixture designs and statistical models for optimizing mobile chromatographic phase and extraction solutions for fingerprint searches. Chemometrics and Intelligent Laboratory Systems, 2007, 89, 82-89.	3.5	8

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163	QTAIM Chargeâ€“Charge Fluxâ€“Dipole Flux Interpretation of Electronegativity and Potential Models of the Fluorochloromethane Mean Dipole Moment Derivatives. Journal of Physical Chemistry A, 2011, 115, 12572-12581.	2.5	8
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