Roy E Bruns

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6335802/publications.pdf

Version: 2024-02-01

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	Unavoidable failure of point charge descriptions of electronic density changes for out-of-plane distortions. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 271, 120891.	3.9	5
2	Electronic Distribution of S_N2 IRC and TS Structures: Infrared Intensities of Imaginary Frequencies. Journal of Chemical Theory and Computation, 2022, 18, 2437-2447.	5.3	4
3	Exogenous application of bioregulators in Coffea arabica beans during ripening: Investigation of UVâ€“Visible and NIR mixture design-fingerprints using AComDim-ICA. Microchemical Journal, 2022, 181, 107702.	4.5	2
4	AC/DC Analysis: Broad and Comprehensive Approach to Analyze Infrared Intensities at the Atomic Level. Journal of Physical Chemistry A, 2021, 125, 3219-3229.	2.5	5
5	Time dependent berry maturation for planting density levels in Coffea arabica L. beans: Mixture design-fingerprinting using near-infrared transmittance spectroscopy. Journal of Food Composition and Analysis, 2021, 97, 103795.	3.9	8
6	Atomic charge and atomic dipole modeling of gas-phase infrared intensities of fundamental bands for out-of-plane CH and CF bending vibrations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 251, 119393.	3.9	5
7	Topological electron density properties at critical points along aromatic rings as reactivity and regioselectivity descriptors in electrophilic substitutions. Journal of Physical Organic Chemistry, 2021, 34, e4252.	1.9	3
8	Are â€œGAPT Chargesâ€•Really Just Charges?. Journal of Chemical Information and Modeling, 2021, 61, 3881-3890.	5.4	15
9	Electrostatics Explains the Reverse Lewis Acidity of BH3 and Boron Trihalides: Infrared Intensities and a Relative Energy Gradient (REG) Analysis of IQA Energies. Journal of Physical Chemistry A, 2021, 125, 8615-8625.	2.5	7
10	Ecometabolic mixture design-fingerprints from exploratory multi-block data analysis in Coffea arabica beans from climate changes: Elevated carbon dioxide and reduced soil water availability. Food Chemistry, 2021, 362, 129716.	8.2	7
11	Authentication of carioca common bean cultivars (Phaseolus vulgaris L.) using digital image processing and chemometric tools. Food Chemistry, 2021, 364, 130349.	8.2	8
12	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
13	Factorial design fingerprint discrimination of Coffea arabica beans under elevated carbon dioxide and limited water conditions. Talanta, 2020, 209, 120591.	5.5	14
14	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
15	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
16	FT-IR biomarkers of sexual dimorphism in yerba-mate plants: Seasonal and light accessibility effects. Microchemical Journal, 2020, 158, 105329.	4.5	12
17	Revisiting the negative dipole moment derivatives of HNgX molecules. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	0
18	Variation of the Distribution of Atmospheric n-Alkanes Emitted by Different Fuelsâ€™ Combustion. Atmosphere, 2020, 11, 643.	2.3	11

#	Article	IF	Citations
19	A tribute to Professor Ronei J. Poppi, a pioneer of multivariate calibration in South America and a prolific mentor of chemometricians in Brazil. Journal of Chemometrics, 2020, 34, e3284.	1.3	1
20	Quantum chemical intensity determinations of overlapped gas phase infrared bands. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 230, 118067.	3.9	2
21	QTAIM Atomic Charge and Polarization Parameters and Their Machine-Learning Transference among Boron-Halide Molecules. Journal of Physical Chemistry A, 2020, 124, 3407-3416.	2.5	3
22	Special issue â€“ VIII Brazilian Chemometrics Workshop. Food Chemistry, 2019, 273, 1-2.	8.2	2
23	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
24	Infrared Intensification and Hydrogen Bond Stabilization: Beyond Point Charges. Journal of Physical Chemistry A, 2019, 123, 6482-6490.	2.5	12
25	Integrated Chemometric Approach to Optimize Sample Preparation for Detecting Metabolic Changes Provoked by Abiotic Stress in Coffea arabica L. Leaf Fingerprints. Journal of the Brazilian Chemical Society, 2019, , .	0.6	2
26	Photodiode array chromatographic-spectrophotometric metabolite quantification for yerba-mate plant sexual dimorphism differentiation. Microchemical Journal, 2019, 151, 104218.	4.5	7
27	FTIR and dispersive gas phase absolute infrared intensities of hydrocarbon fundamental bands. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 214, 1-6.	3.9	7
28	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
29	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
30	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
31	Seasonal changes and solvent effects on fractionated functional food component yields from Mikania laevigata leaves. Food Chemistry, 2019, 273, 151-158.	8.2	14
32	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
33	Atomic Polarizations, Not Charges, Determine CH Out-of-Plane Bending Intensities of Benzene Molecules. Journal of Physical Chemistry A, 2018, 122, 9833-9841.	2.5	8
34	PARAFAC HPLC-DAD metabolomic fingerprint investigation of reference and crossed coffees. Food Research International, 2018, 113, 9-17.	6.2	15
35	Probing the robustness of the charge-charge transfer-dipolar polarization model and infrared intensities. Journal of Molecular Modeling, 2018, 24, 182.	1.8	3
36	FTIR and dispersive gas phase fundamental infrared intensities of the fluorochloromethanes: Comparison with QCISD/cc-pVTZ results. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 205, 269-275.	3.9	8

#	Article	IF	Citations
37	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
38	Mixed oil formulations enriched in essential fatty acids and reduced ratio of n-6/n-3. European Journal of Lipid Science and Technology, 2017, 119, 1600400.	1.5	4
39	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
40	Atomic polarizations necessary for coherent infrared intensity modeling with theoretical calculations. Journal of Chemical Physics, 2017, 146, 134107.	3.0	8
41	Multivariate Optimization of Chlorogenic Acid Extraction From Brazilian Coffee. Food Analytical Methods, 2017, 10, 2943-2951.	2.6	8
42	Quantum Theory of Atoms in Molecules Chargeâ€“Charge Transferâ€“Dipolar Polarization Classification of Infrared Intensities. Journal of Physical Chemistry A, 2017, 121, 8115-8123.	2.5	3
43	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
44	Optimization of frying oil composition rich in essential fatty acids by mixture design. LWT - Food Science and Technology, 2017, 84, 795-803.	5.2	7
45	Infrared spectral evidence and DFT calculations of hydrogen-bonding and molecular structures of acetogenins. Journal of Molecular Structure, 2017, 1130, 174-180.	3.6	4
46	Irrigation and Light Access Effects on Coffea arabica L. Leaves by FTIRâ€‘Chemometric Analysis. Journal of the Brazilian Chemical Society, 2017, , .	0.6	3
47	Chemometric Analysis of UV Characteristic Profile and Infrared Fingerprint Variations ofCoffea arabicaGreen Beans under Different Space Management Treatments. Journal of the Brazilian Chemical Society, 2016, , .	0.6	1
48	Review of Experimental GAPT and Infrared Atomic Charges in Molecules. Journal of the Brazilian Chemical Society, 2016, , .	0.6	5
49	Comment on â€œPropionaldehyde infrared crossâ€“sections and band strengthsâ€•by B. KÃ¶roÄŸlu et al.. Journal of Quantitative Spectroscopy and Radiative Transfer, 2016, 179, 137-138.	2.3	0
50	Characteristic infrared intensities of carbonyl stretching vibrations. Physical Chemistry Chemical Physics, 2016, 18, 17575-17585.	2.8	17
51	Revisiting the integrated infrared intensities and atomic polar tensors of the boron trihalides. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 164, 123-127.	3.9	1
52	QTAIM-Based Characteristic Group Infrared Intensities of Amino Acids and Their Transference to Peptides. Journal of Physical Chemistry A, 2016, 120, 8387-8399.	2.5	6
53	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
54	Dynamic atomic contributions to infrared intensities of fundamental bands. Physical Chemistry Chemical Physics, 2015, 17, 30378-30388.	2.8	16

#	Article	IF	Citations
55	Multivariate optimisation of ICP OES instrumental parameters for Pb/Ba/Sb measurement in gunshot residues. Microchemical Journal, 2015, 120, 58-63.	4.5	28
56	Spectroscopic and Chromatographic Fingerprint Analysis of Composition Variations inCoffea arabicaLeaves Subject to Different Light Conditions and Plant Phenophases. Journal of the Brazilian Chemical Society, 2014, , .	0.6	3
57	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
58	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
59	Open column, reversed-phase high-performance liquid chromatography with diode array detection and chemometric strategy for investigation of metabolic fingerprints of complex systems. Analytical Methods, 2014, 6, 9567-9574.	2.7	3
60	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
61	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
62	Coreâ€“valence correlation effects on IR calculations: the BF3 and BCl3 cases. Journal of Molecular Modeling, 2014, 20, 2333.	1.8	2
63	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
64	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
65	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
66	QTAIM chargeâ€“charge fluxâ€“dipole flux models for the fundamental infrared intensities of BF3 and BCl3. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 116, 136-142.	3.9	6
67	Optimization of Electrophoretic Separations of Thirteen Phenolic Compounds using Single Peak Responses and an Interactive Computer Technique. Journal of the Brazilian Chemical Society, 2013, , .	0.6	1
68	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
69	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
70	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
71	Basis set selection for the calculation of the IR fundamental intensities for 1,1-C2H2F2 and F2CO. Journal of Molecular Structure, 2012, 1009, 49-54.	3.6	5
72	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

#	Article	IF	Citations
73	Mixture designs for exploring class diversity and metabolite fingerprinting: An efficient column chromatographic strategy. Analytica Chimica Acta, 2011, 702, 288-294.	5.4	11
74	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
75	Chemometrics optimization of carbohydrate separations in six food matrices by micellar electrokinetic chromatography with anionic surfactant. Talanta, 2011, 85, 237-244.	5.5	17
76	EstatÃstica aplicada Ã quÃmica: dez dÃºvidas comuns. Quimica Nova, 2011, 34, 888-892.	0.3	9
77	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
78	Comparison of Emission of Dioxins and Furans from Gasohol- and Ethanol-Powered Vehicles. Journal of the Air and Waste Management Association, 2011, 61, 1344-1352.	1.9	3
79	Mixture Design and Response Surface Analysis of Densification of Silicon Carbide Ceramics with (SiO₂â€“Dy₂O₃â€“Al₂O₃) Additives. International Journal of Applied Ceramic Technology, 2010, 7, 493-501.	2.1	3
80	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
81	Optimisation of a CE method for caffeine analysis in decaffeinated coffee. Food Chemistry, 2010, 120, 1155-1161.	8.2	47
82	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
83	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
84	Coupled cluster and configuration interaction quantum calculations of infrared fundamental intensities. International Journal of Quantum Chemistry, 2010, 110, 2029-2036.	2.0	4
85	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
86	Synthesis Optimization of Hydroxymethylnitrofurazone, an Antichagasic Candidate, Using 32 Factorial Design. Letters in Organic Chemistry, 2010, 7, 191-195.	0.5	5
87	Simultaneous determination of first-line anti-tuberculosis drugs by capillary zone electrophoresis using direct UV detection. Talanta, 2010, 82, 333-339.	5.5	45
88	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
89	Emission of polycyclic aromatic hydrocarbons from gasohol and ethanol vehicles. Atmospheric Environment, 2009, 43, 648-654.	4.1	54
90	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

#	Article	IF	Citations
91	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
92	Factorial design preparation of transparent conducting oxide thin films. Thin Solid Films, 2009, 517, 2886-2891.	1.8	7
93	Quantum Theory Atoms in Molecules Chargeâ^'Charge Fluxâ^'Dipole Flux Models for the Infrared Intensities of Benzene and Hexafluorobenzene. Journal of Physical Chemistry A, 2009, 113, 7972-7978.	2.5	5
94	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
95	Statistical mixture designâ€"Varimax factor optimization for selective compound extraction from plant material. Analytica Chimica Acta, 2008, 613, 48-55.	5.4	19
96	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
97	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
98	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
99	A Glimpse of Recent Developments in Brazilian Analytical Chemistry. Analytical Letters, 2008, 41, 1494-1546.	1.8	1
100	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
101	Eucalyptus Tar Pitch Substitution of Phenol in the Preparation of Novolak-Type Resins Cured with Hexamethylenetetramine. Bulletin of the Chemical Society of Japan, 2008, 81, 1528-1533.	3.2	1
102	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
103	Mineral composition of wheat flour consumed in Brazilian cities. Journal of the Brazilian Chemical Society, 2008, 19, 935-942.	0.6	36
104	Technological aspects for restructuring concentrated pineapple pulp. LWT - Food Science and Technology, 2007, 40, 759-765.	5.2	8
105	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
106	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
107	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
108	Study of the reaction conditions for the hydrodechlorination of pentachlorophenol on palladium catalysts. Chemical Engineering Journal, 2007, 131, 59-64.	12.7	13

#	Article	IF	Citations
109	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
110	Statistical designs and response surface techniques for the optimization of chromatographic systems. Journal of Chromatography A, 2007, 1158, 2-14.	3.7	493
111	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
112	Box-Behnken design: An alternative for the optimization of analytical methods. Analytica Chimica Acta, 2007, 597, 179-186.	5.4	2,226
113	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
114	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
115	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
116	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
117	ConseqÃ¼Ãªncias da anÃ¡lise incorreta de experimentos blocados. Quimica Nova, 2007, 30, 436-440.	0.3	0
118	PrecisÃ£o dos mÃ©todos refratomÃ©tricos para anÃ¡lise de umidade em mel. Food Science and Technology, 2007, 27, 328-332.	1.7	0
119	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
120	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
121	25 anos de quimiometria no Brasil. Quimica Nova, 2006, 29, 1401-1406.	0.3	22
122	Electrospray ionization mass spectrometry fingerprinting of perfumes: rapid classification and counterfeit detection. Rapid Communications in Mass Spectrometry, 2006, 20, 3654-3658.	1.5	21
123	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
124	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
125	Chapter 3 Changing everything at the same time. Data Handling in Science and Technology, 2005, 25, 83-145.	3.1	2
126	Chapter 2 When the situation is normal. Data Handling in Science and Technology, 2005, 25, 9-81.	3.1	1

#	Article	IF	Citations
127	32 Factorial design and response surface analysis optimization of N-carboxybutylchitosan synthesis. Carbohydrate Polymers, 2005, 59, 37-42.	10.2	30
128	Split-plot designs and normal probability graphs for the optimization of chemical systems. Analytica Chimica Acta, 2005, 544, 206-212.	5.4	7
129	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
130	Chapter 6 Exploring the response surface. Data Handling in Science and Technology, 2005, 25, 245-312.	3.1	4
131	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
132	Dioxins and furans in the atmosphere of SÃ£o Paulo City, Brazil. Chemosphere, 2005, 58, 1391-1398.	8.2	35
133	InfluÃªncia do material e volume do porta-amostra na determinaÃ§Ã£o termogravimÃ©trica do teor de cinzas em mel. Quimica Nova, 2005, 28, 713-715.	0.3	2
134	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
135	Reducing the number of experiments in split-plot optimization designs. Journal of the Brazilian Chemical Society, 2004, 15, 241-245.	0.6	1
136	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
137	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
138	Characterization of monofloral honeys by ash contents through a hierarchical design. Journal of Food Composition and Analysis, 2004, 17, 737-747.	3.9	27
139	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
140	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
141	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
142	An application of chemometric techniques to analyze the effects of the wave function modifications on the intermolecular stretching frequencies of the hydrogen-bonded complexes. Chemometrics and Intelligent Laboratory Systems, 2004, 70, 157-163.	3.5	6
143	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
144	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

#	Article	IF	Citations
145	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
146	Optimization of thermogravimetric analysis of ash content in honey. Journal of the Brazilian Chemical Society, 2004, 15, 797-802.	0.6	18
147	Simulation of Aerated Lagoon Using Artificial Neural Networks and Multivariate Regression Techniques. Applied Biochemistry and Biotechnology, 2003, 106, 437-450.	2.9	3
148	Title is missing!. Journal of Applied Electrochemistry, 2003, 33, 1069-1075.	2.9	14
149	The infrared fundamental intensities and polar tensor of CH3NC. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 37-45.	3.9	1
150	Artifact evidence in carbonyl compound sampling using the enclosure technique with cuvette system. Journal of Environmental Monitoring, 2003, 5, 795.	2.1	3
151	Core Ionization Energies, Mean Dipole Moment Derivatives, and Simple Potential Models for B, N, O, F, P, Cl, and Br Atoms in Molecules. Journal of Physical Chemistry A, 2002, 106, 1824-1833.	2.5	6
152	The linear relationship between Koopmans' and hydrogen bond energies for some simple carbonyl molecules. Journal of the Brazilian Chemical Society, 2002, 13, 800.	0.6	7
153	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
154	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
155	The infrared intensities and polar tensors of the fluorochloromethanes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 255-264.	3.9	5
156	The infrared fundamental intensities and polar tensor of allene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 1369-1375.	3.9	4
157	Principal component analysis in studies of substituent-induced chemical shifts of 1,4-disubstituted benzenes. Magnetic Resonance in Chemistry, 2001, 39, 316-322.	1.9	7
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	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
160	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
161	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
162	Title is missing!. Biotechnology Letters, 2001, 23, 1963-1969.	2.2	56

#	Article	IF	Citations
163	An electronegativity model for the fundamental infrared intensities of the halomethanes. Computational and Theoretical Chemistry, 2001, 539, 149-157.	1.5	6
164	Some New Data for Metal Desorption on Inorganicâ€“Organic Hybrid Materials. Journal of Colloid and Interface Science, 2000, 227, 66-70.	9.4	14
165	Simple potential models for carbon 1s ionization energies using infrared mean dipole moment derivatives. Journal of Electron Spectroscopy and Related Phenomena, 2000, 107, 211-219.	1.7	5
166	Atomic Mean Dipole Moment Derivatives and GAPT Charges. Journal of Physical Chemistry A, 2000, 104, 5320-5327.	2.5	40
167	3D-WHIM pattern recognition study for bisamidines. A structure-property relationship study. Journal of the Brazilian Chemical Society, 2000, 11, 393-397.	0.6	5
168	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
169	CCl4: mean dipole moment derivatives and core electron binding energies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 2215-2219.	3.9	6
170	Factorial design â€“ principal component regression calculation of fundamental vibrational frequencies. Computational and Theoretical Chemistry, 1999, 464, 163-170.	1.5	0
171	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
172	A Simple Potential Model Criterion for the Quality of Atomic Charges. Journal of Physical Chemistry A, 1999, 103, 4918-4924.	2.5	31
173	Estudo comparativo da seletividade de um mÃ©todo cinÃ©tico-catalÃtico: a determinaÃ§Ã£o de Cr(VI) pela oxidaÃ§Ã£o da o-dianisidina pelo perÃ³xido de hidrogÃªnio. Quimica Nova, 1999, 22, 189-193.	0.3	2
174	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
175	Title is missing!. World Journal of Microbiology and Biotechnology, 1998, 14, 487-490.	3.6	21
176	A statistical approach of density functional effects on the vibrational frequencies and infrared intensities of CH3F. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1998, 54, 831-841.	3.9	1
177	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
178	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
179	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
180	Core Electron Energies, Infrared Intensities, and Atomic Charges. Journal of the American Chemical Society, 1997, 119, 4224-4231.	13.7	38

#	Article	IF	Citations
181	Application of statistical mixture models for ternary polymer blends. Journal of the Brazilian Chemical Society, 1997, 8, 587-595.	0.6	1
182	Transferability of thecis-andtrans-Dichloroethylene Atomic Polar Tensors. Journal of Physical Chemistry A, 1997, 101, 6293-6298.	2.5	7
183	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
184	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
185	Factorial design and principal component analyses of the vibrational frequencies and infrared intensities of methane and silane. Computational and Theoretical Chemistry, 1997, 394, 187-196.	1.5	7
186	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
187	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
188	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
189	Infrared vibrational intensities and polar tensors of the carbonyl and thiocarbonyl halides. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 2115-2128.	3.9	7
190	A chemometric analysis ofab initio vibrational frequencies and infrared intensities of methyl fluoride. Journal of Computational Chemistry, 1996, 17, 167-177.	3.3	25
191	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
192	Is statistical lack of fit a reliable criterion for chemical complexity?. Chemometrics and Intelligent Laboratory Systems, 1996, 33, 159-166.	3.5	5
193	Carbon 1s Electron Ionization Energies and Infrared Intensities of the Chlorofluoromethanes. Journal of the Brazilian Chemical Society, 1996, 7, 497-503.	0.6	4
194	Principal component analysis of the methylene chloride polar tensors. Computational and Theoretical Chemistry, 1995, 335, 113-121.	1.5	4
195	Hydrogen-Bonded Dimers of CH3OCH2CH2OH: Ab Initio Structures and Multivariate Analysis. The Journal of Physical Chemistry, 1995, 99, 634-638.	2.9	6
196	Infrared Vibrational Intensities and Polar Tensors of the Fluorochloromethanes. The Journal of Physical Chemistry, 1995, 99, 11357-11364.	2.9	6
197	Electronegativity Models for the Infrared Vibrational Intensities of the Halomethanes. Journal of the American Chemical Society, 1995, 117, 4144-4150.	13.7	15
198	Optimizing the Enzymatic Maceration of Foliole PurÃ©e from Hard Pieces of Hearts of Palm (Euterpe) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	3.1	3

#	Article	IF	Citations
199	Principal component analysis of the13C NMR shifts of norbornyl derivatives. IIâ€"tetracyclic dodecane derivatives. Magnetic Resonance in Chemistry, 1993, 31, 247-253.	1.9	2
200	A principal component analysis of the methyl fluoride polar tensors. Computational and Theoretical Chemistry, 1993, 282, 81-89.	1.5	14
201	Catalytic determination of molybdenum (VI) in plants using mono-segmented continuous-flow analysis and spectrophotometric detection. Analyst, The, 1993, 118, 213.	3.5	20
202	A multivariate statistical analysis of the composition of rainwater near CubatÃ£o, SP, Brazil. Environmental Pollution, 1993, 79, 225-233.	7.5	17
203	Principal component analyses of the methyl chloride, bromide, and iodide polar tensors. The Journal of Physical Chemistry, 1993, 97, 4354-4359.	2.9	8
204	Principal component analysis of the cis- and trans-difluoroethylene polar tensors. The Journal of Physical Chemistry, 1993, 97, 6161-6166.	2.9	17
205	Effects of Reagent Addition Sequence on the Analytical Response of the Mo(VI)-catalysed oxidation of Iodide by Hydrogen Peroxide. Journal of the Brazilian Chemical Society, 1993, 4, 128-132.	0.6	2
206	Polymer-polymer miscibility evaluation by acoustic emission. Die Makromolekulare Chemie Rapid Communications, 1992, 13, 45-53.	1.1	10
207	Principal component analysis of the polar tensors of difluoromethane and difluoromethane-d2. The Journal of Physical Chemistry, 1991, 95, 9716-9720.	2.9	14
208	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
209	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
210	Principal component analysis of dipole moment derivative signs of chloroform. Journal of Computational Chemistry, 1991, 12, 885-890.	3.3	25
211	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
212	Dipole moment derivative signs, polar tensors, and vibrational intensities of hexafluoroethane. The Journal of Physical Chemistry, 1989, 93, 2957-2959.	2.9	3
213	molecular orbital calculations of the polar tensors and vibrational intensities of HC3N. Journal of Molecular Structure, 1988, 175, 355-358.	3.6	4
214	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
215	An electronegativity model for vibrational intensities of substituted methanes. Journal of Chemical Physics, 1988, 89, 1887-1891.	3.0	16
216	The atomic polar tensors, effective charges and vibrational intensities of the CHnN (n = 3, 5, 7 and 9) molecules. Journal of Molecular Structure, 1986, 142, 209-212.	3.6	3

#	Article	IF	Citations
217	Similarity transference of molecular parameters. I. The atomic polar tensors of cyanoacetylene. Journal of Chemical Physics, 1986, 85, 4515-4523.	3.0	9
218	Transferability of the cis- and trans-difluoroethylene polar tensors. The Journal of Physical Chemistry, 1985, 89, 4979-4983.	2.9	13
219	A fast procedure for standard additions in flow injection analysis. Analytica Chimica Acta, 1985, 171, 337-343.	5.4	31
220	A polar tensor calculation of the infrared absorption intensities of formyl fluoride. Spectrochimica Acta Part A: Molecular Spectroscopy, 1983, 39, 1111-1115.	0.1	1
221	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
222	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
223	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
224	Gâ€sum rule separation of overlapping vibrational bands. Journal of Chemical Physics, 1982, 76, 821-824.	3.0	4
225	The determination of experimental signs of dipole moment derivatives: G sum rule analysis of allene. Journal of Molecular Spectroscopy, 1981, 87, 298-299.	1.2	1
226	Flow injection systems with inductively-coupled argon plasma atomic emission spectrometry. Analytica Chimica Acta, 1981, 130, 243-255.	5.4	76
227	Dipole moment derivatives, polar tensors, and effective charges of allene. The Journal of Physical Chemistry, 1980, 84, 2808-2813.	2.9	7
228	Polar tensors, effective charges, and vibrational intensities of the M(CO)6 (M = chromium,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 307 Td 84, 3593-3597.	2.9	5
229	On the use of F and G sum rules as error indicators of experimental vibrational intensity data: The CHxD3â^'xBr molecules. Journal of Chemical Physics, 1979, 70, 5338-5339.	3.0	3
230	G sum rule applications for the vibrational intensities of the hydrocarbons. Journal of Chemical Physics, 1979, 71, 5042.	3.0	14
231	Experimental determination of relative signs of dipole moment derivatives: HCN and DCN. Journal of Chemical Physics, 1978, 68, 847-851.	3.0	30
232	F and G intensity sum rule applications: the CHxD4â^'x molecules. Journal of Chemical Physics, 1978, 69, 4147-4148.	3.0	9
233	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
234	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

#	Article	IF	Citations
235	Gâ€intensity sum rule applications: XY3 molecules. Journal of Chemical Physics, 1978, 68, 5448-5450.	3.0	9
236	Mean dipole moment derivatives, atomic anisotropies, and effective charges of diatomic hydrides. Journal of Chemical Physics, 1978, 68, 880-885.	3.0	21
237	The signs of the dipole moment derivatives of carbonic dibromide and predicted derivatives for carbonothioic dibromide. The Journal of Physical Chemistry, 1978, 82, 1908-1911.	2.9	2
238	On the structure of the benzene-chlorine complex: a CNDO study. Journal of Molecular Structure, 1977, 36, 121-126.	3.6	8
239	A molecular orbital study of the chloramphenicol family of drugs: A preliminary report. International Journal of Quantum Chemistry, 1977, 12, 357-362.	2.0	0
240	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
241	The theoretical calculation of polar tensors and dipole moment derivatives: BF3 and Bcl3. Journal of Chemical Physics, 1976, 64, 3053-3056.	3.0	11
242	Mean dipole moment derivatives and anisotropies of X2CY molecules. Journal of Chemical Physics, 1976, 64, 3084-3085.	3.0	11
243	Dipole moment derivatives, polar tensors, and effective charges of ammonia and phosphine. The Journal of Physical Chemistry, 1976, 80, 2768-2770.	2.9	12
244	Polar tensors and effective charges of carbonic dibromide. The Journal of Physical Chemistry, 1975, 79, 1880-1882.	2.9	8
245	An empirical determination of the infrared intensities of Cl2CS. Journal of Molecular Structure, 1975, 26, 124-125.	3.6	4
246	Donorâ€"acceptor interactions of substituted benzenes with molecular chlorine and carbon disulfide. Journal of Molecular Structure, 1975, 29, 211-223.	3.6	8
247	The polar tensors, effective charges, and infrared intensities of X2CY molecules. Journal of Chemical Physics, 1975, 62, 3235-3239.	3.0	28
248	Molecular orbital studies of the dipole moments of methyl substituted amines, phosphines, and their borane adducts. Inorganica Chimica Acta, 1975, 14, 271-280.	2.4	7
249	Regularities in calculated dipole moment derivatives of first row diatomic hydrides. Journal of Chemical Physics, 1974, 61, 1779-1781.	3.0	8
250	The carbonyl vibration in Î±-Group IV metal ketones. Journal of Organometallic Chemistry, 1973, 56, 131-140.	1.8	18
251	Resonant Raman effect and charge distribution in the TCNE-benzene charge transfer complex. Chemical Physics Letters, 1973, 21, 357-359.	2.6	5
252	Dipole moment derivatives and vibrational intensities of BCl3. Journal of Chemical Physics, 1973, 59, 4362-4366.	3.0	7

#	Article	IF	Citations
253	CNDO calculation of dipole moment derivatives and infrared intensities of formaldehyde. Journal of Chemical Physics, 1973, 58, 2585-2592.	3.0	29
254	Vibrational intensities of F2CS and Cl2CS. Journal of Chemical Physics, 1973, 58, 1855-1860.	3.0	19
255	Vibrational intensities of F2CO, Cl2CO, and Br2CO. Journal of Chemical Physics, 1973, 58, 1849-1854.	3.0	20
256	CNDO Calculation of Dipole Moment Derivatives and Infrared Intensities of C6H6 and C6F6. Journal of Chemical Physics, 1972, 57, 324-331.	3.0	35
257	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
258	CNDO Calculation of Dipoleâ€Moment Derivatives and Infrared Intensities of BF3. Journal of Chemical Physics, 1971, 55, 5401-5404.	3.0	21
259	Vibrational Intensities in F2CO: Some Corrections. Journal of Chemical Physics, 1971, 55, 2890-2894.	3.0	29
260	Calculated Dipoleâ€Moment Functions and the Infrared Intensities of HCN and N2O. Journal of Chemical Physics, 1970, 53, 1413-1417.	3.0	53
261	A theoretical study of the bond-bond interaction force constant in XF2 molecules. Theoretica Chimica Acta, 1969, 14, 232-241.	0.8	2
262	Calculation of the Vibrational Intensities of F2CO. Journal of Chemical Physics, 1969, 50, 3811-3812.	3.0	31
263	Photoinduced reactions in solid carbon suboxide. Inorganic Chemistry, 1967, 6, 318-320.	4.0	2
264	Influence of Seasonality and Sunlight Effects on Rollinia mucosa Leaves Fingerprint. Journal of the Brazilian Chemical Society, 0, , .	0.6	2
265	Understanding the Hydrogen-Bond by means of Infrared intensities: A Quantum Theory CCTDP approach.. , 0, , .		0