Marcel Maeder

List of Publications by Year in Descending Order

152 papers	6,776 citations	36 h-index	80 g-index
155 ext. papers	7,110 ext. citations	4.4 avg, IF	5.67 L-index

#	Paper	IF	Citations
152	Chemical model-based optimization of a sensor array for simultaneous determination of glucose and fructose. *Microchemical Journal*, **2021**, 172, 106944	4.8	
151	Heterogeneous catalysts for the hydrogenation of amine/alkali hydroxide solvent captured CO2 to formate: A review **2021**, 11, 807-823		3
150	Using chemical modeling for designing of optimal pH sensor based on analytical sensitivity enhancement. *Microchemical Journal*, **2021**, 168, 106450	4.8	2
149	Generalized indicator-based determination of solution pH. *Analytica Chimica Acta*, **2020**, 1109, 90-97	6.6	4
148	Turning Routine Data into Systems Insight: Multivariate Analysis of Water Quality Dynamics in a Major Drinking Water Reservoir. *Environmental Modeling and Assessment*, **2020**, 25, 565-579	2	
147	On the avoidance of crossing of singular values in the evolving factor analysis. *Journal of Chemometrics*, **2020**, 34, e3217	1.6	2
146	A perspective on modeling evolution. *Journal of Chemometrics*, **2020**, 34, e3205	1.6	1
145	Using chemometrics tools to gain detailed molecular information on chemical processes. *Journal of Chemometrics*, **2020**, 34, e3207	1.6	
144	Multiset Data Analysis: Extended Multivariate Curve Resolution **2020**, 305-336		5
143	Kinetic Absorption of CO2 into Blended Ammonia (NH3) Solutions with a New Cyclic Amine 4-Aminomethyltetrahydropyran (4-AMTHP). *Energy & Fuels*, **2019**, 33, 5377-5383	4.1	3
142	Activity-based analysis of potentiometric pH titrations. *Analytica Chimica Acta*, **2019**, 1075, 49-56	6.6	1
141	A chemical equilibrium modelling strategy for tuning the apparent equilibrium constants of the chemical systems. *Analytica Chimica Acta*, **2019**, 1049, 29-37	6.6	7
140	Topics in chemometrics, TIC 2017, a personal report. *Journal of Chemometrics*, **2018**, 32, e3025	1.6	
139	Handling Different Spatial Resolutions in Image Fusion by Multivariate Curve Resolution-Alternating Least Squares for Incomplete Image Multisets. *Analytical Chemistry*, **2018**, 90, 6757-6765	7.8	21
138	Kinetics of the reversible reaction of CO2(aq) with taurate in aqueous solution **2018**, 8, 672-685		
137	Handling of highly coeluted chromatographic peaks by multivariate curve resolution for a complex bioanalytical problem: Quantitation of selected corticosteroids and mycophenolic acid in human plasma. *Talanta*, **2018**, 187, 1-12	6.2	11
136	Quantum chemical computation-based strategy for alternating least squares initialization in multivariate curve resolution analysis of spectral-pH data. *Microchemical Journal*, **2018**, 140, 183-188	4.8	3

135	PHOSPHATE ESTER HYDROLYSIS PROMOTED BY AN AMIDOPYRIDINE CARBOXYLATE COMPLEX. *Rasayan Journal of Chemistry*, **2018**, 11, 894-903	1.6	2
134	Insights into the Chemical Mechanism for CO(aq) and H in Aqueous Diamine Solutions - An Experimental Stopped-Flow Kinetic and H/C NMR Study of Aqueous Solutions of N,N-Dimethylethylenediamine for Postcombustion CO Capture. *Environmental Science & Technology*, **2018**, 52, 9116-9126	10.3	17
133	Development and Evaluation of a Novel Method for Determining Absorbent Composition in Aqueous Ammonia-Based CO2 and SO32− and SO42− Loaded Capture Process Solutions via FT-IR Spectroscopy. *Energy & Fuels*, **2018**, 32, 8563-8570	4.1	4
132	The thermodynamic formation constants for iron(III) thiocyanate complexes at zero ionic strength. *Inorganica Chimica Acta*, **2017**, 466, 249-253	2.7	7
131	A new matching image preprocessing for image data fusion. *Chemometrics and Intelligent Laboratory Systems*, **2017**, 164, 32-42	3.8	19
130	Investigation of metal ion additives on the suppression of ammonia loss and CO2 absorption kinetics of aqueous ammonia-based CO2 capture. *International Journal of Greenhouse Gas Control*, **2017**, 56, 165-172	4.2	13
129	The Henry Coefficient of CO2 in the MEA-CO2-H2O System. *Energy Procedia*, **2017**, 114, 1841-1847	2.3	3
128	Kinetic and Equilibrium Reactions of a New Heterocyclic Aqueous 4-Aminomethyltetrahydropyran (4-AMTHP) Absorbent for Post Combustion Carbon Dioxide (CO2) Capture Processes. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 9200-9206	8.3	6
127	The determination of the Henry's Coefficient of reactive gases – An example of CO2 in aqueous solutions of monoethanolamine (MEA). *Chemical Engineering Science*, **2017**, 173, 474-482	4.4	2
126	Enhanced target factor analysis. *Analytica Chimica Acta*, **2016**, 911, 35-41	6.6	2
125	A review of recent methods for the determination of ranges of feasible solutions resulting from soft modelling analyses of multivariate data. *Analytica Chimica Acta*, **2016**, 911, 1-13	6.6	95
124	A new approach to the equilibrium study of iron(III) thiocyanates which accounts for the kinetic instability of the complexes particularly observable under high thiocyanate concentrations. *Inorganica Chimica Acta*, **2016**, 445, 155-159	2.7	16
123	Model-based analysis of coupled equilibrium-kinetic processes: indirect kinetic studies of thermodynamic parameters using the dynamic data. *Analyst, The*, **2015**, 140, 3121-35	5	4
122	Catalysis of CO2 absorption in aqueous solution by vanadate and sulfate and their application to post combustion capture. *International Journal of Greenhouse Gas Control*, **2015**, 36, 60-65	4.2	7
121	The effect of piperazine (PZ) on CO2 absorption kinetics into aqueous ammonia solutions at 25.0°C. *International Journal of Greenhouse Gas Control*, **2015**, 36, 135-143	4.2	19
120	A study of bovine and human carbonic anhydrases as a model enzyme system for CO2 hydration in post combustion capture. *International Journal of Greenhouse Gas Control*, **2015**, 37, 85-89	4.2	8
119	A speciation study of sulfur(iv) in aqueous solution. *Dalton Transactions*, **2014**, 43, 2147-52	4.3	16
118	CO2 Absorption into Aqueous Solutions Containing 3-Piperidinemethanol: CO2 Mass Transfer, Stopped-Flow Kinetics, 1H/13C NMR, and Vapor−Liquid Equilibrium Investigations. *Industrial & Engineering Chemistry Research*, **2014**, 53, 16715-16724	3.9	14

117	Protonation Constants and Thermodynamic Properties of Amino Acid Salts for CO2 Capture at High Temperatures. *Industrial & Engineering Chemistry Research*, **2014**, 53, 12848-12855	3.9	11
116	[1.1.1]Cryptand: directions for its use as a variable-pH kinetic molecular device. *New Journal of Chemistry*, **2014**, 38, 561-567	3.6	4
115	Catalysis of CO absorption in aqueous solution by inorganic oxoanions and their application to post combustion capture. *Environmental Science & Technology*, **2014**, 48, 4623-9	10.3	23
114	Chemometric Tools for Image Analysis **2014**, 57-110		3
113	Amino acids/NH3 Mixtures for CO2 Capture: Effect of Neutralization Methods on CO2 Mass Transfer and NH3 Vapour Loss. *Energy Procedia*, **2014**, 63, 773-780	2.3	12
112	Parametric Investigation of Chemical Equilibrium in Mixed Aqueous Amine Systems for CO2 Capture Processes: Impact of Amine Protonation and Reaction Enthalpies on CO2 Absorption Capacity, Cyclic Capacity, and Absorption Enthalpies. *Energy Procedia*, **2014**, 63, 1818-1826	2.3	3
111	A Novel Process Concept for the Capture of CO2 and SO2 Using a Single Solvent and Column. *Energy Procedia*, **2014**, 63, 703-714	2.3	12
110	An SO 2 tolerant process for CO 2 capture. *International Journal of Greenhouse Gas Control*, **2014**, 31, 205-213	4.2	9
109	Chemometrics and data fitting. *Journal of Chemometrics*, **2013**, 27, n/a-n/a	1.6	1
108	Determination and visualization of rotational ambiguity in four-component systems. *Analytica Chimica Acta*, **2013**, 796, 20-6	6.6	34
107	Multivariate linear regression with missing values. *Analytica Chimica Acta*, **2013**, 796, 38-41	6.6	2
106	The Role of SO2 in the Chemistry of Amine-based CO2 Capture in PCC. *Energy Procedia*, **2013**, 37, 1262-1266	2.56	8
105	A simple chemical model to represent CO2 amine H2O vapour liquid-equilibria. *International Journal of Greenhouse Gas Control*, **2013**, 17, 215-224	4.2	35
104	Effect of Sarcosinate on the Absorption Kinetics of CO2 into Aqueous Ammonia Solution. *Industrial & Engineering Chemistry Research*, **2013**, 52, 6382-6389	3.9	11
103	Toward the understanding of chemical absorption processes for post-combustion capture of carbon dioxide: electronic and steric considerations from the kinetics of reactions of CO2(aq) with sterically hindered amines. *Environmental Science & Technology*, **2013**, 47, 1163-9	10.3	67
102	Reactions of CO2 with aqueous piperazine solutions: formation and decomposition of mono- and dicarbamic acids/carbamates of piperazine at 25.0 C. *Journal of Physical Chemistry A*, **2013**, 117, 806-13	2.8	47
101	Protonation constants and thermodynamic properties of amines for post combustion capture of CO2. *Journal of Chemical Thermodynamics*, **2012**, 51, 97-102	2.9	65
100	Toward rational design of amine solutions for PCC applications: the kinetics of the reaction of CO2(aq) with cyclic and secondary amines in aqueous solution. *Environmental Science & Technology*, **2012**, 46, 7422-9	10.3	59

99	Kinetics of the reversible reaction of CO2(aq) and HCO3(-) with sarcosine salt in aqueous solution. *Journal of Physical Chemistry A*, **2012**, 116, 10276-84	2.8	23
98	The reduction of rotational ambiguity in soft-modeling by introducing hard models. *Analytica Chimica Acta*, **2012**, 709, 32-40	6.6	35
97	Investigations of primary and secondary amine carbamate stability by 1H NMR spectroscopy for post combustion capture of carbon dioxide. *Journal of Chemical Thermodynamics*, **2012**, 54, 183-191	2.9	62
96	Comprehensive kinetic and thermodynamic study of the reactions of CO2(aq) and HCO3(-) with monoethanolamine (MEA) in aqueous solution. *Journal of Physical Chemistry A*, **2011**, 115, 14340-9	2.8	81
95	Resolution of rotational ambiguity for three-component systems. *Analytical Chemistry*, **2011**, 83, 836-41	7.8	81
94	A calorimetric study of carbamate formation. *Journal of Chemical Thermodynamics*, **2011**, 43, 664-669	2.9	29
93	Kinetics of the reversible reaction of CO2(aq) with ammonia in aqueous solution. *Journal of Physical Chemistry A*, **2011**, 115, 6405-12	2.8	67
92	Prediction of the overall enthalpy of CO2 absorption in aqueous amine systems from experimentally determined reaction enthalpies. *Energy Procedia*, **2011**, 4, 1542-1549	2.3	15
91	A systematic investigation of carbamate stability constants by 1H NMR. *International Journal of Greenhouse Gas Control*, **2011**, 5, 396-400	4.2	41
90	Synthesis, characterization, and crystal structure of a tricadmium complex of 3,4-diamino-5-methyl-1,2,4-triazole. *Journal of Coordination Chemistry*, **2011**, 64, 105-114	1.6	20
89	Complexation of the N,N?,O-donor ligand N-trans-(2?-hydroxycyclohexyl)-2-aminomethylpyridine. *Journal of Coordination Chemistry*, **2011**, 64, 3637-3651	1.6	4
88	Conjoint Analysis of Kinetic and Equilibrium Data for Mechanistic Elucidation in Polynuclear Complexation Reactions, Exemplified by Metal(II) Helicate Complex Formation. *Australian Journal of Chemistry*, **2010**, 63, 141	1.2	
87	Synthesis and metal(II) ion complexation of pyridine-2,6-diamides incorporating amino alcohols. *Journal of Coordination Chemistry*, **2010**, 63, 2400-2418	1.6	2
86	Comprehensive study of the hydration and dehydration reactions of carbon dioxide in aqueous solution. *Journal of Physical Chemistry A*, **2010**, 114, 1734-40	2.8	171
85	Complexation of Constrained Ligands Piperazine, N-substituted Piperazines, and Thiomorpholine. *Australian Journal of Chemistry*, **2009**, 62, 1196	1.2	4
84	Symmetrical diamides based on 2,6-bis(methoxycarbonyl)pyridine: Syntheses and metal ion binding studies. *Journal of Heterocyclic Chemistry*, **2009**, 46, 243-250	1.9	3
83	Tutorial: the modelling of chemical processes. *Analytica Chimica Acta*, **2009**, 647, 31-9	6.6	5
82	Molecular interactions between amine and carbonate species in aqueous solution kinetics and thermodynamics. *Energy Procedia*, **2009**, 1, 995-1002	2.3	4

81	Calculation and meaning of feasible band boundaries in multivariate curve resolution of a two-component system. *Analytical Chemistry*, **2009**, 81, 2115-22	7.8	82
80	Kinetics and mechanism of carbamate formation from CO2(aq), carbonate species, and monoethanolamine in aqueous solution. *Journal of Physical Chemistry A*, **2009**, 113, 5022-9	2.8	171
79	Carbon dioxide postcombustion capture: a novel screening study of the carbon dioxide absorption performance of 76 amines. *Environmental Science & Technology*, **2009**, 43, 6427-33	10.3	415
78	Simulation of Enthalpy and Capacity of CO2 Absorption by Aqueous Amine Systems. *Industrial & Engineering Chemistry Research*, **2008**, 47, 2002-2009	3.9	157
77	Use of local rank-based spatial information for resolution of spectroscopic images. *Journal of Chemometrics*, **2008**, 22, 291-298	1.6	74
76	Aminoalcohols incorporating a piperazine ring: Synthesis, complexation of a hexadentate ligand and DNA cleavage capability of copper(II) complexes. *Inorganica Chimica Acta*, **2007**, 360, 2403-2410	2.7	3
75	Cyclic polyamines via a molybdenum(0) templated Mannich-type reaction. *Transition Metal Chemistry*, **2007**, 32, 287-291	2.1	2
74	Complexation kinetics of copper(II) and nickel(II) with macrocycles: identification of an outer-sphere chelate effect. *Inorganic Chemistry*, **2007**, 46, 4002-9	5.1	20
73	On rotational ambiguity in model-free analyses of multivariate data. *Journal of Chemometrics*, **2006**, 20, 302-310	1.6	98
72	Model-Based Analysis for Kinetic and Equilibrium Investigations. *Critical Reviews in Analytical Chemistry*, **2006**, 36, 199-209	5.2	35
71	Advances in the modelling and analysis of complex and industrial processes. *Chemometrics and Intelligent Laboratory Systems*, **2006**, 82, 75-82	3.8	14
70	Tutorial on the fitting of kinetics models to multivariate spectroscopic measurements with non-linear least-squares regression. *Chemometrics and Intelligent Laboratory Systems*, **2006**, 81, 149-164	3.8	69
69	Equilibrium modeling of mixtures of methanol and water. *Applied Spectroscopy*, **2005**, 59, 329-34	3.1	14
68	Abstracting reliable parameters from time-correlated single photon counting experiments. *Journal of Photochemistry and Photobiology A: Chemistry*, **2005**, 175, 221-225	4.7	2
67	Palladium(II) as a versatile template for the formation of tetraaza macrocycles via Mannich-type reactions. *Inorganica Chimica Acta*, **2005**, 358, 3227-3235	2.7	7
66	Modeling of batch reactions with in situ spectroscopic measurements and calorimetry. *Journal of Chemometrics*, **2005**, 19, 329-340	1.6	25
65	Synthesis of a Four-Strand N2O2-Donor Ligand and its Transition Metal Complexation Probed by Electrospray Ionisation Mass Spectrometry. *Transition Metal Chemistry*, **2004**, 29, 505-510	2.1	2
64	Spectroscopic imaging and chemometrics: a powerful combination for global and local sample analysis. *TrAC - Trends in Analytical Chemistry*, **2004**, 23, 70-79	14.6	152

63	Metal-directed synthesis of a chiral acyclic pentaamine and pendant-arm macrocyclic hexaamine derived from an amino acid. *Inorganica Chimica Acta*, **2004**, 357, 557-570	2.7	9
62	Calibration-free estimates of batch process yields and detection of process upsets using in situ spectroscopic measurements and nonisothermal kinetic models: 4-(dimethylamino)pyridine-catalyzed esterification of butanol. *Analytical Chemistry*, **2004**, 76, 2575-82	7.8	31
61	Octahedral Complexes of a Mixed N,N,O-Donor Ligand N-trans-(2'-hydroxycyclohexyl)-2-aminomethylpyridine. *Australian Journal of Chemistry*, **2004**, 57, 483	1.2	7
60	Comparative stability constants for metal ions with tetraazamacrocycles of various ring sizes carrying a single amine or carboxylate pendant group. *Transition Metal Chemistry*, **2003**, 28, 460-463	2.1	4
59	Analyses of three-way data from equilibrium and kinetic investigations. *Analytica Chimica Acta*, **2003**, 490, 99-108	6.6	22
58	Analysis of reactions in aqueous solution at non-constant pH: no more buffers?. *Physical Chemistry Chemical Physics*, **2003**, 5, 2836	3.6	49
57	Application of a combination of hard and soft modeling for equilibrium systems to the quantitative analysis of pH-modulated mixture samples. *Analytical Chemistry*, **2003**, 75, 641-7	7.8	84
56	Geometrical isomerism in octahedral complexes arising from the presence of a fused ring on a triaza macrocycle. *Dalton Transactions*, **2003**, 2188	4.3	6
55	Simulation of Complex Chemical Kinetics. *Bioinorganic Reaction Mechanisms*, **2003**, 5, 39-46		4
54	Isomers of 1,4,8,11-Tetraazacyclotetradecane-6,13-dicarboxylate Characterized as Cobalt(III) Complexes. *Australian Journal of Chemistry*, **2003**, 56, 679	1.2	5
53	Hard-modelled trilinear decomposition (HTD) for an enhanced kinetic multicomponent analysis. *Journal of Chemometrics*, **2002**, 16, 218-227	1.6	21
52	Rank annihilation correction for the amendment of instrumental inconsistencies. *Analytica Chimica Acta*, **2002**, 464, 249-259	6.6	21
51	An electrospray ionization mass spectrometry study of the nitroprusside□ation□hiolate system. *Dalton Transactions RSC*, **2002**, 3649-3655		13
50	Excited state acidity of bifunctional compounds. *Physical Chemistry Chemical Physics*, **2002**, 4, 3383-3389	3.6	7
49	Target transform fitting: a new method for the non-linear fitting of multivariate data with separable parameters. *Journal of Chemometrics*, **2001**, 15, 511-522	1.6	19
48	Exhaustive evolving factor analysis (E-EFA). *Journal of Chemometrics*, **2001**, 15, 475-484	1.6	24
47	Application of a novel resolution approach combining soft- and hard-modelling features to investigate temperature-dependent kinetic processes. *Analytica Chimica Acta*, **2001**, 442, 337-350	6.6	82
46	Formation kinetics of pendant arm polyamine macrocycles with copper(II). *Dalton Transactions RSC*, **2001**, 2376-2382		17

45	Resolving factor analysis. *Analytical Chemistry*, **2001**, 73, 1587-94	7.8	57
44	Metal-directed synthesis routes to a 16-membered tetraazamacrocycle with two pendant primary amine groups. *Inorganica Chimica Acta*, **2000**, 306, 1-5	2.7	8
43	Metol□a stereo-rigid four-strand motif for alkali and alkaline earth metal ion coordination. *Inorganic Chemistry Communication*, **2000**, 3, 410-414	3.1	2
42	Combining hard- and soft-modelling to solve kinetic problems. *Chemometrics and Intelligent Laboratory Systems*, **2000**, 54, 123-141	3.8	259
41	Characterization of the Minor cis Isomer of a Dipendant Polyamino Acid Macrocycle as a Dimeric Nickel(II) Complex. *Australian Journal of Chemistry*, **2000**, 53, 517	1.2	6
40	New developments for the numerical analysis of spectrophotometric titrations. *Polyhedron*, **1999**, 18, 3227-3232	2.7	10
39	Hard modelling of spectroscopic measurements. Applications in non-ideal industrial reaction systems. *Chemometrics and Intelligent Laboratory Systems*, **1999**, 46, 221-230	3.8	31
38	Kinetics of Heavy Metal Ion Adsorption on to, and Proton Release from, Electrolytic Manganese Dioxide. *Adsorption Science and Technology*, **1998**, 16, 39-50	3.6	4
37	Variation in the Adsorption of Lead(II) by a Range of Electrolytic Manganese Dioxides: Chemometric Examination of Correlation with Physical Properties. *Adsorption Science and Technology*, **1997**, 15, 583-592	3.6	
36	Outer-sphere complex formation and catalysis of adenosine 5?-triphosphate hydrolysis with polyammonium cations: kinetics employing an attenuated total reflectance infrared method. *Inorganica Chimica Acta*, **1997**, 254, 353-359	2.7	3
35	Hydrogenolysis of a pendant alcohol dithiadiazamacrocycle. Crystal structure of the 6-amino-6-methyl-1, 11-dithia-4,8-diazacyclotetradecane hydrogenolysis product as a chlorocobalt(III) complex. *Inorganica Chimica Acta*, **1997**, 261, 197-200	2.7	4
34	Analysis of non-isothermal kinetic measurements. *Analytica Chimica Acta*, **1997**, 337, 73-81	6.6	42
33	Second order global analysis: the evaluation of series of spectrophotometric titrations for improved determination of equilibrium constants. *Analytica Chimica Acta*, **1997**, 353, 381-393	6.6	99
32	A Saturated Heterocycle Formed from Ethane-1,2-diamine, Formaldehyde and Nitroethane: Crystal Structure of 6-Methyl-6-nitro-1,4-bis(2?-nitropropan-1?-yl)-1,4-diazacycloheptane. *Australian Journal of Chemistry*, **1997**, 50, 241	1.2	2
31	Macrocycle Formation Through Carbon Acid - Formaldehyde Condensation Reactions of Bis(propane-1,2-diamine)- and Bis(2-methylpropane-1,2-diamine)-copper(II) Ions. *Australian Journal of Chemistry*, **1997**, 50, 529	1.2	24
30	"Swollen" Macrocycles: Palladium(II)-Directed Template Syntheses of Pendant-Arm 14-, 16-, and 18-Membered Macrocycles. *Inorganic Chemistry*, **1996**, 35, 4961-4966	5.1	17
29	Nickel(II) complexes of 15-membered tetraaza macrocycles with a primary amine or carboxylate pendant: structural characterization of a one-dimensional chain compound. *Inorganica Chimica Acta*, **1996**, 246, 65-71	2.7	8
28	Isolation of and metal ion selection by geometric isomers of a pendant-arm macrotricyclic hexaamine. *Polyhedron*, **1996**, 15, 3157-3162	2.7	2

27	ATR-IR Spectroscopy for the Investigation of Solution Reaction Kinetics: Hydrolysis of Trimethyl Phosphate. *Applied Spectroscopy*, **1995**, 49, 1789-1792	3.1	11
26	A spectrophotometric method for the quantification of outer-sphere coordination: A bicyclic ammonium cation with the hexacyanocobaltate(III) anion. *Supramolecular Chemistry*, **1994**, 3, 261-266	1.8	
25	Second-order globalisation for the determination of activation parameters in kinetics. *Analytica Chimica Acta*, **1994**, 298, 193-201	6.6	61
24	Outer-sphere coordination of polycyanometallate anions with polyammonium macrocycles: A spectrophotometric study. *Inorganica Chimica Acta*, **1994**, 227, 71-77	2.7	6
23	Molecular Oxygen, Superoxide, and Peroxide as Ligands in a CoN5 Complex. *Inorganic Chemistry*, **1994**, 33, 3135-3140	5.1	12
22	METAL-DIRECTED MACROCYCLIZATION REACTIONS INVOLVING FORMALDEHYDE, AMINES AND MONO- OR BI-FUNCTIONAL METHYLENE COMPOUNDS. *Reviews in Inorganic Chemistry*, **1993**, 13, 199-232	2.4	27
21	Polyamine complexation. Stability constants for metal ion complexation of 5-(4?-amino-2?-azabutane)-5-methyl-3,7-diazanonane-1,9-diamine. *Polyhedron*, **1991**, 10, 409-413	2.7	7
20	Macromonocycle formation from copper(II)- or nickel(II)-directed condensation of linear tetraamines and formaldehyde with various nitro-carbon acids. *Polyhedron*, **1990**, 9, 2227-2231	2.7	15
19	Principal components regression in practice. An evaluation of EMD battery activity from X-ray diffraction patterns. *TrAC - Trends in Analytical Chemistry*, **1990**, 9, 303-308	14.6	1
18	Coordination of the "pendant-arm" macrocycle 6,13-diamino-6,13-dimethyl-1,4,8,11-tetraazacyclotetradecane to chromium(III). Crystal structure and physical properties of the hexacoordinated complex ion. *Inorganic Chemistry*, **1990**, 29, 3208-3213	5.1	17
17	Nonlinear least-squares fitting of multivariate absorption data. *Analytical Chemistry*, **1990**, 62, 2220-2224	7.8	367
16	Energy-Minimized Structures and Calculated and Experimental Isomer distributions in the hexaamine-cobalt(III) system [Co(L)2]3+ with the chiral facially-coordinating triamine (l = butane-1,2,4-triamine). *Helvetica Chimica Acta*, **1989**, 72, 1029-1037	2	16
15	Evolving factor analysis, a new multivariate technique in chromatography. *Chemometrics and Intelligent Laboratory Systems*, **1988**, 3, 205-213	3.8	191
14	Computerized data acquisition and data reduction in spectrophotometric analysis of metal ion complexes. Part 1. General considerations and data acquisition. *TrAC - Trends in Analytical Chemistry* , **1988**, 7, 111-113	14.6	19
13	Computerized data acquisition and data reduction in spectrophotometric analysis Part 2: numerical analysis with and without an underlying chemical model. *TrAC - Trends in Analytical Chemistry*, **1988**, 7, 147-150	14.6	10
12	Evolving factor analysis for the resolution of overlapping chromatographic peaks. *Analytical Chemistry*, **1987**, 59, 527-530	7.8	604
11	Evolving Factor Analysis. *Comments on Inorganic Chemistry*, **1987**, 6, 41-60	3.9	29
10	Quantification of a known component in an unknown mixture. *Analytica Chimica Acta*, **1987**, 193, 287-298	5.6	92

9	The resolution of overlapping chromatographic peaks by evolving factor analysis. *Analytica Chimica Acta*, **1986**, 181, 287-291	6.6	207
8	Calculation of equilibrium constants from multiwavelength spectroscopic data-III Model-free analysis of spectrophotometric and ESR titrations. *Talanta*, **1985**, 32, 1133-9	6.2	388
7	Calculation of equilibrium constants from multiwavelength spectroscopic data--II: SPECFIT: two user-friendly programs in basic and standard FORTRAN 77. *Talanta*, **1985**, 32, 257-64	6.2	369
6	Calculation of equilibrium constants from multiwavelength spectroscopic data-I Mathematical considerations. *Talanta*, **1985**, 32, 95-101	6.2	466
5	Absorption and MCD spectral studies of the decaammine(.mu.-dinitrogen-N,N')diosmium(5+) mixed-valence ion. *Journal of the American Chemical Society*, **1985**, 107, 2167-2171	16.4	19
4	Copper(II) complexes with linear pentadentate chelators. *Inorganic Chemistry*, **1984**, 23, 3724-3730	5.1	29
3	Spectrophotometric data reduction by eigenvector analysis for equilibrium and kinetic studies and a new method of fitting exponentials. *Analytica Chimica Acta*, **1980**, 122, 303-313	6.6	19
2	General non-linear least-squares program for the numerical treatment of spectrophotometric data on a single-precision game computer. *Talanta*, **1980**, 27, 1037-46	6.2	41
1	Chemometric Tools for Image Analysis65-109		36