Klaus Neymeyr

List of Publications by Year
in descending order

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80	1,205	394421	414414
papers	citations	19 h-index	32 g-index

81	81	81	531
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	5.4	118
2	A fast polygon inflation algorithm to compute the area of feasible solutions for threeâ€component systems. I: concepts and applications. Journal of Chemometrics, 2013, 27, 106-116.	1.3	70
3	A geometric theory for preconditioned inverse iteration III: A short and sharp convergence estimate for generalized eigenvalue problems. Linear Algebra and Its Applications, 2003, 358, 95-114.	0.9	65
4	A fast polygon inflation algorithm to compute the area of feasible solutions for threeâ€component systems. II: Theoretical foundation, inverse polygon inflation, and FACâ€PACK implementation. Journal of Chemometrics, 2014, 28, 633-644.	1.3	53
5	Exploring Between the Extremes: Conversionâ€Dependent Kinetics of Phosphiteâ€Modified Hydroformylation Catalysis. Chemistry - A European Journal, 2012, 18, 8780-8794.	3.3	52
6	A geometric theory for preconditioned inverse iteration I: Extrema of the Rayleigh quotient. Linear Algebra and Its Applications, 2001, 322, 61-85.	0.9	51
7	A Comparative Inâ€…Situ HPâ€FTIR Spectroscopic Study of Biâ€and Monodentate Phosphiteâ€Modified Hydroformylation. ChemCatChem, 2010, 2, 287-295.	3.7	48
8	Reduction of the rotational ambiguity of curve resolution techniques under partial knowledge of the factors. Complementarity and coupling theorems. Journal of Chemometrics, 2012, 26, 526-537.	1.3	44
9	On generalized Borgen plots. I: From convex to affine combinations and applications to spectral dataSpectra. Journal of Chemometrics, 2015, 29, 420-433.	1.3	34
10	Modelâ€free multivariate curve resolution combined with modelâ€based kinetics: algorithm and applications. Journal of Chemometrics, 2012, 26, 538-548.	1.3	33
11	A geometric theory forpreconditioned inverse iterationII: Convergence estimates. Linear Algebra and Its Applications, 2001, 322, 87-104.	0.9	32
12	An Operando FTIR Spectroscopic and Kinetic Study of Carbon Monoxide Pressure Influence on Rhodiumâ€Catalyzed Olefin Hydroformylation. Chemistry - A European Journal, 2014, 20, 11921-11931.	3.3	31
13	Investigation into the Equilibrium of Iridium Catalysts for the Hydroformylation of Olefins by Combining In Situ High-Pressure FTIR and NMR Spectroscopy. ACS Catalysis, 2014, 4, 2097-2108.	11.2	30
14	On the area of feasible solutions and its reduction by the complementarity theorem. Analytica Chimica Acta, 2014, 828, 17-26.	5.4	27
15	Pure component spectral recovery and constrained matrix factorizations: concepts and applications. Journal of Chemometrics, 2010, 24, 67-74.	1.3	25
16	Multilevel Method for Mixed Eigenproblems. SIAM Journal of Scientific Computing, 2002, 23, 2141-2164.	2.8	24
17	A posteriori error estimation for elliptic eigenproblems. Numerical Linear Algebra With Applications, 2002, 9, 263-279.	1.6	24
18	Soft constraints for reducing the intrinsic rotational ambiguity of the area of feasible solutions. Chemometrics and Intelligent Laboratory Systems, 2015, 149, 140-150.	3.5	23

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19	A geometric theory for preconditioned inverse iteration applied to a subspace. Mathematics of Computation, 2001, 71, 197-217.	2.1	19
20	Gradient Flow Approach to Geometric Convergence Analysis of Preconditioned Eigensolvers. SIAM Journal on Matrix Analysis and Applications, 2009, 31, 621-628.	1.4	18
21	A ray casting method for the computation of the area of feasible solutions for multicomponent systems: Theory, applications and FACPACK-implementation. Analytica Chimica Acta, 2017, 960, 40-52.	5.4	18
22	On the ambiguity of the reaction rate constants in multivariate curve resolution for reversible first-order reaction systems. Analytica Chimica Acta, 2016, 927, 21-34.	5.4	17
23	Simultaneous construction of dual Borgen plots. I: The case of noiseâ€free data. Journal of Chemometrics, 2017, 31, e2954.	1.3	17
24	Investigating the effect of flexible constraints on the accuracy of selfâ€modeling curve resolution methods in the presence of perturbations. Journal of Chemometrics, 2016, 30, 252-267.	1.3	16
25	Multi-objective optimization for an automated and simultaneous phase and baseline correction of NMR spectral data. Journal of Magnetic Resonance, 2018, 289, 132-141.	2.1	16
26	The Influence of Substituents in Diphosphine Ligands on the Hydrogenation Activity and Selectivity of the Corresponding Rhodium Complexes as Exemplified by ButiPhane. ChemCatChem, 2012, 4, 81-88.	3.7	15
27	On the Analysis and Computation of the Area of Feasible Solutions for Two-, Three-, and Four-Component Systems. Data Handling in Science and Technology, 2016, , 135-184.	3.1	15
28	Simultaneous construction of dual Borgen plots. II: Algorithmic enhancement for applications to noisy spectral data. Journal of Chemometrics, 2018, 32, e3012.	1.3	13
29	Does the signal contribution function attain its extrema on the boundary of the area of feasible solutions?. Chemometrics and Intelligent Laboratory Systems, 2020, 196, 103887.	3.5	13
30	Peak group analysis for the extraction of pure component spectra. Journal of the Iranian Chemical Society, 2016, 13, 191-205.	2.2	12
31	Probing relaxation models by means of Fast Field-Cycling relaxometry, NMR spectroscopy and molecular dynamics simulations: Detailed insight into the translational and rotational dynamics of a protic ionic liquid. Journal of Molecular Liquids, 2020, 319, 114207.	4.9	12
32	Insights into the translational and rotational dynamics of cations and anions in protic ionic liquids by means of NMR fast-field-cycling relaxometry. Physical Chemistry Chemical Physics, 2021, 23, 2663-2675.	2.8	12
33	Convergence Analysis of Gradient Iterations for the Symmetric Eigenvalue Problem. SIAM Journal on Matrix Analysis and Applications, 2011, 32, 443-456.	1.4	11
34	A Geometric Convergence Theory for the Preconditioned Steepest Descent Iteration. SIAM Journal on Numerical Analysis, 2012, 50, 3188-3207.	2.3	11
35	?Neglect of Diatomic Differential Overlap? in nonempirical quantum chemical orbital theories. I. On the justification of the neglect of diatomic differential overlap approximation. International Journal of Quantum Chemistry, 1995, 53, 515-518.	2.0	10
36	Solute-induced perturbation of methanolâ€“water association. RSC Advances, 2015, 5, 71102-71108.	3.6	10

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37	How To Apply the Complementarity and Coupling Theorems in MCR Methods: Practical Implementation and Application to the Rhodium-Catalyzed Hydroformylation. ACS Catalysis, 2014, 4, 2836-2843.	11.2	8
38	Mechanistic insights into dehydrocoupling of amine boranes using dinuclear zirconocene complexes. Catalysis Science and Technology, 2021, 11, 4034-4050.	4.1	8
39	A geometric theory for preconditioned inverse iteration IV: On the fastest convergence cases. Linear Algebra and Its Applications, 2006, 415, 114-139.	0.9	7
40	On an SVDâ€free approach to the complementarity and coupling theory A note on the elimination of unknowns in sums of dyadic products. Journal of Chemometrics, 2016, 30, 30-36.	1.3	7
41	On the Set of Solutions of the Nonnegative Matrix Factorization Problem. SIAM Journal on Matrix Analysis and Applications, 2018, 39, 1049-1069.	1.4	7
42	Unraveling VEALYL Amyloid Formation Using Advanced Vibrational Spectroscopy and Microscopy. Biophysical Journal, 2020, 119, 87-98.	0.5	7
43	On the restrictiveness of equality constraints in multivariate curve resolution. Chemometrics and Intelligent Laboratory Systems, 2020, 199, 103942.	3.5	7
44	Towards operando IRâ€•and UVâ€visâ€Spectroâ€Electrochemistry: A Comprehensive Matrix Factorisation Study on Sensitive and Transient Molybdenum and Tungsten Monoâ€Dithiolene Complexes**. Chemistry Methods, 2021, 1, 22-35.	3.8	7
45	Determination of Unstable Limit Cycles in Chaotic Systems by the Method of Unrestricted Harmonic Balance. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1991, 46, 499-502.	1.5	6
46	A note on Inverse Iteration. Numerical Linear Algebra With Applications, 2005, 12, 1-8.	1.6	6
47	Convergence Theory for Preconditioned Eigenvalue Solvers in a Nutshell. Foundations of Computational Mathematics, 2017, 17, 713-727.	2.5	6
48	Introducing the monotonicity constraint as an effective chemistry-based condition in self-modeling curve resolution. Chemometrics and Intelligent Laboratory Systems, 2019, 190, 22-32.	3.5	6
49	Multivariate curve resolution methods and the design of experiments. Journal of Chemometrics, 2020, 34, e3159.	1.3	6
50	?Neglect of Diatomic Differential Overlap? in nonempirical quantum chemical orbital theories. V. A calculus of error concerning the justification of the neglect of diatomic differential overlap (NDDO) approximation. International Journal of Quantum Chemistry, 1995, 53, 553-568.	2.0	5
51	On generalized Borgen plots II: The lineâ€moving algorithm and its numerical implementation. Journal of Chemometrics, 2016, 30, 636-650.	1.3	5
52	How noise affects the band boundaries in multivariate curve resolution. Chemometrics and Intelligent Laboratory Systems, 2022, 220, 104472.	3.5	5
53	?Neglect of Diatomic Differential Overlap? in nonempirical quantum chemical orbital theories. II. A polynomial expansion for ??1/2 in terms of Legendre and Chebyshev polynomials. International Journal of Quantum Chemistry, 1995, 53, 519-535.	2.0	4
54	?Neglect of Diatomic Differential Overlap? in nonempirical quantum chemical orbital theories. III. On the spectrum of the overlap matrix for diatomic molecules over locally orthogonalized basis functions. International Journal of Quantum Chemistry, 1995, 53, 537-540.	2.0	4

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55	?Neglect of Diatomic Differential Overlap? in nonempirical quantum chemical orbital theories. IV. An examination of the justification of the neglect of diatomic differential overlap (NDDO) approximation. International Journal of Quantum Chemistry, 1995, 53, 541-552.	2.0	4
56	On preconditioned eigensolvers and Invertâ€“Lanczos processes. Linear Algebra and Its Applications, 2009, 430, 1039-1056.	0.9	4
57	Comparative multivariate curve resolution study in the area of feasible solutions. Chemometrics and Intelligent Laboratory Systems, 2017, 163, 55-63.	3.5	4
58	Photochemical multivariate curve resolution models for the investigation of photochromic systems under continuous irradiation. Analytica Chimica Acta, 2019, 1053, 32-42.	5.4	4
59	A multi-method chemometric analysis in spectroelectrochemistry: Case study on molybdenum mono-dithiolene complexes. Analytica Chimica Acta, 2021, 1185, 339065.	5.4	4
60	Iterative minimization of the Rayleigh quotient by block steepest descent iterations. Numerical Linear Algebra With Applications, 2014, 21, 604-617.	1.6	3
61	Convergence Analysis of Restarted Krylov Subspace Eigensolvers. SIAM Journal on Matrix Analysis and Applications, 2016, 37, 955-975.	1.4	3
62	Analysis of the ambiguity in the determination of quantum yields from spectral data on a photoinduced isomerization. Chemometrics and Intelligent Laboratory Systems, 2019, 189, 88-95.	3.5	3
63	Application of a new method for simultaneous phase and baseline correction of NMR signals (SINC). Magnetic Resonance in Chemistry, 2020, 58, 260-270.	1.9	3
64	Facile Synthesis of a Stable Sideâ€on Phosphinyne Complex by Redox Driven Intramolecular Cyclisation. Chemistry - A European Journal, 2020, 26, 11492-11502.	3.3	3
65	Cluster robust estimates for block gradient-type eigensolvers. Mathematics of Computation, 2019, 88, 2737-2765.	2.1	2
66	On the Ambiguity Underlying Multivariate Curve Resolution Methods. , 2020, , 199-231.		2
67	On the avoidance of crossing of singular values in the evolving factor analysis. Journal of Chemometrics, 2020, 34, e3217.	1.3	2
68	On the area of feasible solutions for rankâ€deficient problems: I. Introduction of a generalized concept. Journal of Chemometrics, 2021, 35, e3316.	1.3	2
69	A comparative study of MCR-based kinetic analyses for chemical reaction systems with rate constant ambiguities. Chemometrics and Intelligent Laboratory Systems, 2021, 210, 104228.	3.5	2
70	Calculation of lower and upper band boundaries for the feasible solutions of rank-deficient multivariate curve resolution problems. Chemometrics and Intelligent Laboratory Systems, 2022, 226, 104577.	3.5	2
71	A multiresolution approach for the convergence acceleration of multivariate curve resolution methods. Analytica Chimica Acta, 2015, 891, 101-112.	5.4	1
72	A chemometric study in the area of feasible solution of an acidâ€“base titration of N-methyl-6-oxyquinolone. RSC Advances, 2018, 8, 9922-9932.	3.6	1

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73	On the analysis of chromatographic biopharmaceutical data by curve resolution techniques in the framework of the area of feasible solutions. Journal of Chromatography A, 2020, 1627, 461420.	3.7	1
74	Reaction rate ambiguities for perturbed spectroscopic data: Theory and implementation. Analytica Chimica Acta, 2020, 1137, 170-180.	5.4	1
75	Characterization of the unimodality constraint as an effective chemistry-based condition in resolving of chemical processes data. Microchemical Journal, 2021, 160, 105615.	4.5	1
76	On the signal contribution function with respect to different norms. Journal of Chemometrics, 2021, 35, e3363.	1.3	1
77	Model-based signal tracking in the quantitative analysis of time series of NMR spectra. Journal of Magnetic Resonance, 2022, 339, 107212.	2.1	1
78	On properties of EFA plots. Journal of Chemometrics, 2021, 35, .	1.3	1
79	Simplified Non-Empirical Unrestricted Hartree-Fock Approximation (SUHF) for the Calculation of Electronic Ground State Properties of Molecules with Closed and Open Valence Shells. II. Diatomic Molecules. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1993, 48, 834-840.	1.5	0
80	On optimal step-length gradient eigensolvers. Proceedings in Applied Mathematics and Mechanics, 2011, 11, 749-750.	0.2	0