

Klaus Neymeyr

List of Publications by Year in descending order

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Version: 2024-02-01

80
papers

1,205
citations

394421

19
h-index

414414

32
g-index

81
all docs

81
docs citations

81
times ranked

531
citing authors

#	ARTICLE	IF	CITATIONS
1	How noise affects the band boundaries in multivariate curve resolution. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2022, 220, 104472.	3.5	5
2	Model-based signal tracking in the quantitative analysis of time series of NMR spectra. <i>Journal of Magnetic Resonance</i> , 2022, 339, 107212.	2.1	1
3	Calculation of lower and upper band boundaries for the feasible solutions of rank-deficient multivariate curve resolution problems. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2022, 226, 104577.	3.5	2
4	On the area of feasible solutions for rank-deficient problems: I. Introduction of a generalized concept. <i>Journal of Chemometrics</i> , 2021, 35, e3316.	1.3	2
5	Characterization of the unimodality constraint as an effective chemistry-based condition in resolving of chemical processes data. <i>Microchemical Journal</i> , 2021, 160, 105615.	4.5	1
6	Towards operando IR- and UV-vis-Spectroelectrochemistry: A Comprehensive Matrix Factorisation Study on Sensitive and Transient Molybdenum and Tungsten Mono-dithiolene Complexes**. <i>Chemistry Methods</i> , 2021, 1, 22-35.	3.8	7
7	Insights into the translational and rotational dynamics of cations and anions in protic ionic liquids by means of NMR fast-field-cycling relaxometry. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2663-2675.	2.8	12
8	A comparative study of MCR-based kinetic analyses for chemical reaction systems with rate constant ambiguities. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2021, 210, 104228.	3.5	2
9	On the signal contribution function with respect to different norms. <i>Journal of Chemometrics</i> , 2021, 35, e3363.	1.3	1
10	A multi-method chemometric analysis in spectroelectrochemistry: Case study on molybdenum mono-dithiolene complexes. <i>Analytica Chimica Acta</i> , 2021, 1185, 339065.	5.4	4
11	Mechanistic insights into dehydrocoupling of amine boranes using dinuclear zirconocene complexes. <i>Catalysis Science and Technology</i> , 2021, 11, 4034-4050.	4.1	8
12	On properties of EFA plots. <i>Journal of Chemometrics</i> , 2021, 35, .	1.3	1
13	Multivariate curve resolution methods and the design of experiments. <i>Journal of Chemometrics</i> , 2020, 34, e3159.	1.3	6
14	Application of a new method for simultaneous phase and baseline correction of NMR signals (SINC). <i>Magnetic Resonance in Chemistry</i> , 2020, 58, 260-270.	1.9	3
15	Does the signal contribution function attain its extrema on the boundary of the area of feasible solutions?. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2020, 196, 103887.	3.5	13
16	On the analysis of chromatographic biopharmaceutical data by curve resolution techniques in the framework of the area of feasible solutions. <i>Journal of Chromatography A</i> , 2020, 1627, 461420.	3.7	1
17	On the Ambiguity Underlying Multivariate Curve Resolution Methods. , 2020, , 199-231.		2
18	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. <i>Journal of Molecular Liquids</i> , 2020, 319, 114207.	4.9	12

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19	Reaction rate ambiguities for perturbed spectroscopic data: Theory and implementation. <i>Analytica Chimica Acta</i> , 2020, 1137, 170-180.	5.4	1
20	Unraveling VEALYL Amyloid Formation Using Advanced Vibrational Spectroscopy and Microscopy. <i>Biophysical Journal</i> , 2020, 119, 87-98.	0.5	7
21	Facile Synthesis of a Stable Side-on Phosphinyne Complex by Redox Driven Intramolecular Cyclisation. <i>Chemistry - A European Journal</i> , 2020, 26, 11492-11502.	3.3	3
22	On the restrictiveness of equality constraints in multivariate curve resolution. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2020, 199, 103942.	3.5	7
23	On the avoidance of crossing of singular values in the evolving factor analysis. <i>Journal of Chemometrics</i> , 2020, 34, e3217.	1.3	2
24	Cluster robust estimates for block gradient-type eigensolvers. <i>Mathematics of Computation</i> , 2019, 88, 2737-2765.	2.1	2
25	Introducing the monotonicity constraint as an effective chemistry-based condition in self-modeling curve resolution. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2019, 190, 22-32.	3.5	6
26	Analysis of the ambiguity in the determination of quantum yields from spectral data on a photoinduced isomerization. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2019, 189, 88-95.	3.5	3
27	Photochemical multivariate curve resolution models for the investigation of photochromic systems under continuous irradiation. <i>Analytica Chimica Acta</i> , 2019, 1053, 32-42.	5.4	4
28	Multi-objective optimization for an automated and simultaneous phase and baseline correction of NMR spectral data. <i>Journal of Magnetic Resonance</i> , 2018, 289, 132-141.	2.1	16
29	Simultaneous construction of dual Borgen plots. II: Algorithmic enhancement for applications to noisy spectral data. <i>Journal of Chemometrics</i> , 2018, 32, e3012.	1.3	13
30	A chemometric study in the area of feasible solution of an acid-base titration of <i>N</i> -methyl-6-oxyquinolone. <i>RSC Advances</i> , 2018, 8, 9922-9932.	3.6	1
31	On the Set of Solutions of the Nonnegative Matrix Factorization Problem. <i>SIAM Journal on Matrix Analysis and Applications</i> , 2018, 39, 1049-1069.	1.4	7
32	Convergence Theory for Preconditioned Eigenvalue Solvers in a Nutshell. <i>Foundations of Computational Mathematics</i> , 2017, 17, 713-727.	2.5	6
33	Comparative multivariate curve resolution study in the area of feasible solutions. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2017, 163, 55-63.	3.5	4
34	A ray casting method for the computation of the area of feasible solutions for multicomponent systems: Theory, applications and FACPACK-implementation. <i>Analytica Chimica Acta</i> , 2017, 960, 40-52.	5.4	18
35	Simultaneous construction of dual Borgen plots. I: The case of noise-free data. <i>Journal of Chemometrics</i> , 2017, 31, e2954.	1.3	17
36	Investigating the effect of flexible constraints on the accuracy of self-modeling curve resolution methods in the presence of perturbations. <i>Journal of Chemometrics</i> , 2016, 30, 252-267.	1.3	16

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37	On the ambiguity of the reaction rate constants in multivariate curve resolution for reversible first-order reaction systems. <i>Analytica Chimica Acta</i> , 2016, 927, 21-34.	5.4	17
38	On generalized Borgen plots II: The lineâ€removing algorithm and its numerical implementation. <i>Journal of Chemometrics</i> , 2016, 30, 636-650.	1.3	5
39	Convergence Analysis of Restarted Krylov Subspace Eigensolvers. <i>SIAM Journal on Matrix Analysis and Applications</i> , 2016, 37, 955-975.	1.4	3
40	On an SVDâ€free approach to the complementarity and coupling theory A note on the elimination of unknowns in sums of dyadic products. <i>Journal of Chemometrics</i> , 2016, 30, 30-36.	1.3	7
41	On the Analysis and Computation of the Area of Feasible Solutions for Two-, Three-, and Four-Component Systems. <i>Data Handling in Science and Technology</i> , 2016, , 135-184.	3.1	15
42	Peak group analysis for the extraction of pure component spectra. <i>Journal of the Iranian Chemical Society</i> , 2016, 13, 191-205.	2.2	12
43	A review of recent methods for the determination of ranges of feasible solutions resulting from soft modelling analyses of multivariate data. <i>Analytica Chimica Acta</i> , 2016, 911, 1-13.	5.4	118
44	On generalized Borgen plots. I: From convex to affine combinations and applications to spectral dataSpectra. <i>Journal of Chemometrics</i> , 2015, 29, 420-433.	1.3	34
45	Soft constraints for reducing the intrinsic rotational ambiguity of the area of feasible solutions. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2015, 149, 140-150.	3.5	23
46	A multiresolution approach for the convergence acceleration of multivariate curve resolution methods. <i>Analytica Chimica Acta</i> , 2015, 891, 101-112.	5.4	1
47	Solute-induced perturbation of methanolâ€water association. <i>RSC Advances</i> , 2015, 5, 71102-71108.	3.6	10
48	A fast polygon inflation algorithm to compute the area of feasible solutions for threeâ€component systems. II: Theoretical foundation, inverse polygon inflation, and <i>FACâ€PACK</i> implementation. <i>Journal of Chemometrics</i> , 2014, 28, 633-644.	1.3	53
49	Iterative minimization of the Rayleigh quotient by block steepest descent iterations. <i>Numerical Linear Algebra With Applications</i> , 2014, 21, 604-617.	1.6	3
50	How To Apply the Complementarity and Coupling Theorems in MCR Methods: Practical Implementation and Application to the Rhodium-Catalyzed Hydroformylation. <i>ACS Catalysis</i> , 2014, 4, 2836-2843.	11.2	8
51	An Operando FTIR Spectroscopic and Kinetic Study of Carbon Monoxide Pressure Influence on Rhodiumâ€Catalyzed Olefin Hydroformylation. <i>Chemistry - A European Journal</i> , 2014, 20, 11921-11931.	3.3	31
52	Investigation into the Equilibrium of Iridium Catalysts for the Hydroformylation of Olefins by Combining In Situ High-Pressure FTIR and NMR Spectroscopy. <i>ACS Catalysis</i> , 2014, 4, 2097-2108.	11.2	30
53	On the area of feasible solutions and its reduction by the complementarity theorem. <i>Analytica Chimica Acta</i> , 2014, 828, 17-26.	5.4	27
54	A fast polygon inflation algorithm to compute the area of feasible solutions for threeâ€component systems. I: concepts and applications. <i>Journal of Chemometrics</i> , 2013, 27, 106-116.	1.3	70

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55	A Geometric Convergence Theory for the Preconditioned Steepest Descent Iteration. SIAM Journal on Numerical Analysis, 2012, 50, 3188-3207.	2.3	11
56	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
57	Model-free multivariate curve resolution combined with model-based kinetics: algorithm and applications. Journal of Chemometrics, 2012, 26, 538-548.	1.3	33
58	Exploring Between the Extremes: Conversion-Dependent Kinetics of Phosphite-Modified Hydroformylation Catalysis. Chemistry - A European Journal, 2012, 18, 8780-8794.	3.3	52
59	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
60	On optimal step-length gradient eigensolvers. Proceedings in Applied Mathematics and Mechanics, 2011, 11, 749-750.	0.2	0
61	Convergence Analysis of Gradient Iterations for the Symmetric Eigenvalue Problem. SIAM Journal on Matrix Analysis and Applications, 2011, 32, 443-456.	1.4	11
62	A Comparative In-Situ HP-FTIR Spectroscopic Study of Bi- and Monodentate Phosphite-Modified Hydroformylation. ChemCatChem, 2010, 2, 287-295.	3.7	48
63	Pure component spectral recovery and constrained matrix factorizations: concepts and applications. Journal of Chemometrics, 2010, 24, 67-74.	1.3	25
64	On preconditioned eigensolvers and Invert-Lanczos processes. Linear Algebra and Its Applications, 2009, 430, 1039-1056.	0.9	4
65	Gradient Flow Approach to Geometric Convergence Analysis of Preconditioned Eigensolvers. SIAM Journal on Matrix Analysis and Applications, 2009, 31, 621-628.	1.4	18
66	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
67	A note on Inverse Iteration. Numerical Linear Algebra With Applications, 2005, 12, 1-8.	1.6	6
68	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
69	Multilevel Method for Mixed Eigenproblems. SIAM Journal of Scientific Computing, 2002, 23, 2141-2164.	2.8	24
70	A posteriori error estimation for elliptic eigenproblems. Numerical Linear Algebra With Applications, 2002, 9, 263-279.	1.6	24
71	A geometric theory for preconditioned inverse iteration applied to a subspace. Mathematics of Computation, 2001, 71, 197-217.	2.1	19
72	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

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73	A geometric theory for preconditioned inverse iteration II: Convergence estimates. <i>Linear Algebra and Its Applications</i> , 2001, 322, 87-104.	0.9	32
74	?Neglect of Diatomic Differential Overlap? in nonempirical quantum chemical orbital theories. I. On the justification of the neglect of diatomic differential overlap approximation. <i>International Journal of Quantum Chemistry</i> , 1995, 53, 515-518.	2.0	10
75	?Neglect of Diatomic Differential Overlap? in nonempirical quantum chemical orbital theories. II. A polynomial expansion for $\sqrt{1/2}$ in terms of Legendre and Chebyshev polynomials. <i>International Journal of Quantum Chemistry</i> , 1995, 53, 519-535.	2.0	4
76	?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. <i>International Journal of Quantum Chemistry</i> , 1995, 53, 537-540.	2.0	4
77	?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. <i>International Journal of Quantum Chemistry</i> , 1995, 53, 541-552.	2.0	4
78	?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. <i>International Journal of Quantum Chemistry</i> , 1995, 53, 553-568.	2.0	5
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. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 1993, 48, 834-840.	1.5	0
80	Determination of Unstable Limit Cycles in Chaotic Systems by the Method of Unrestricted Harmonic Balance. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 1991, 46, 499-502.	1.5	6