Rafiqul Gani

List of Publications by Citations

482 papers	12,679 citations	60 h-index	97 g-index
522 ext. papers	13,912 ext. citations	2.8 avg, IF	6.89 L-index

#	Paper	IF	Citations
482	New group contribution method for estimating properties of pure compounds. *AICHE Journal*, **1994**, 40, 1697-1710	3.6	817
481	Group-contribution based estimation of pure component properties. *Fluid Phase Equilibria*, **2001**, 183-184, 183-208	2.5	781
480	Assessment of Recent Process Analytical Technology (PAT) Trends: A Multiauthor Review. *Organic Process Research and Development*, **2015**, 19, 3-62	3.9	251
479	Chemical product design: challenges and opportunities. *Computers and Chemical Engineering*, **2004**, 28, 2441-2457	4	240
478	A group contribution approach to computer-aided molecular design. *AICHE Journal*, **1991**, 37, 1318-1332	3.6	203
477	Estimation of the acentric factor and the liquid molar volume at 298 K using a new group contribution method. *Fluid Phase Equilibria*, **1995**, 103, 11-22	2.5	202
476	Computer aided molecular design: a novel method for optimal solvent selection. *Fluid Phase Equilibria*, **1993**, 82, 47-54	2.5	202
475	Group-contribution+ (GC+) based estimation of properties of pure components: Improved property estimation and uncertainty analysis. *Fluid Phase Equilibria*, **2012**, 321, 25-43	2.5	190
474	A multi-step and multi-level approach for computer aided molecular design. *Computers and Chemical Engineering*, **2000**, 24, 677-683	4	171
473	Design of environmentally benign processes: integration of solvent design and separation process synthesis. *Computers and Chemical Engineering*, **1999**, 23, 1395-1414	4	158
472	A novel framework for simultaneous separation process and product design. *Chemical Engineering and Processing: Process Intensification*, **2004**, 43, 595-608	3.7	154
471	Process intensification: A perspective on process synthesis. *Chemical Engineering and Processing: Process Intensification*, **2010**, 49, 547-558	3.7	150
470	A New Decomposition-Based Computer-Aided Molecular/Mixture Design Methodology for the Design of Optimal Solvents and Solvent Mixtures. *Industrial & Engineering Chemistry Research*, **2005**, 44, 4785-4797	3.9	150
469	Toward the Development and Deployment of Large-Scale Carbon Dioxide Capture and Conversion Processes. *Industrial & Engineering Chemistry Research*, **2016**, 55, 3383-3419	3.9	145
468	Separation process design and synthesis based on thermodynamic insights. *Chemical Engineering Science*, **1995**, 50, 511-530	4.4	143
467	Optimal design of a multi-product biorefinery system. *Computers and Chemical Engineering*, **2011**, 35, 1752-1766	4	130
466	A systematic synthesis framework for extractive distillation processes. *Chemical Engineering Research and Design*, **2008**, 86, 781-792	5.5	128

465	Correlation and prediction of thermal properties and phase behaviour for a class of aqueous electrolyte systems. *Chemical Engineering Science*, **1996**, 51, 3675-3683	4.4	128
464	A computer-aided molecular design framework for crystallization solvent design. *Chemical Engineering Science*, **2006**, 61, 1247-1260	4.4	124
463	Method for selection of solvents for promotion of organic reactions. *Computers and Chemical Engineering*, **2005**, 29, 1661-1676	4	124
462	Computer-aided molecular design with combined molecular modeling and group contribution. *Fluid Phase Equilibria*, **1999**, 158-160, 337-347	2.5	122
461	An integrated computer aided system for integrated design of chemical processes. *Computers and Chemical Engineering*, **1997**, 21, 1135-1146	4	116
460	Phenomena Based Methodology for Process Synthesis Incorporating Process Intensification. *Industrial & Engineering Chemistry Research*, **2013**, 52, 7127-7144	3.9	115
459	Are safe results obtained when the PC-SAFT equation of state is applied to ordinary pure chemicals?. *Fluid Phase Equilibria*, **2010**, 295, 76-92	2.5	109
458	Design of formulated products: A systematic methodology. *AICHE Journal*, **2011**, 57, 2431-2449	3.6	103
457	State-of-the-art and progress in the optimization-based simultaneous design and control for chemical processes. *AICHE Journal*, **2012**, 58, 1640-1659	3.6	98
456	Sustainable process synthesis□ntensification. *Computers and Chemical Engineering*, **2015**, 81, 218-244	4	97
455	Design of sustainable chemical processes: Systematic retrofit analysis generation and evaluation of alternatives. *Chemical Engineering Research and Design*, **2008**, 86, 328-346	5.5	96
454	A strategy for the design and selection of solvents for separation processes.. *Fluid Phase Equilibria*, **1986**, 29, 125-132	2.5	96
453	SustainPro□A tool for systematic process analysis, generation and evaluation of sustainable design alternatives. *Computers and Chemical Engineering*, **2013**, 50, 8-27	4	89
452	Simultaneous design of ionic liquid entrainers and energy efficient azeotropic separation processes. *Computers and Chemical Engineering*, **2012**, 42, 248-262	4	88
451	A generic methodology for processing route synthesis and design based on superstructure optimization. *Computers and Chemical Engineering*, **2017**, 106, 892-910	4	87
450	Estimation of environment-related properties of chemicals for design of sustainable processes: development of group-contribution+ (GC+) property models and uncertainty analysis. *Journal of Chemical Information and Modeling*, **2012**, 52, 2823-39	6.1	86
449	Optimal design of microalgae-based biorefinery: Economics, opportunities and challenges. *Applied Energy*, **2015**, 150, 69-79	10.7	85
448	Biorefining: Computer aided tools for sustainable design and analysis of bioethanol production. *Chemical Engineering Research and Design*, **2009**, 87, 1171-1183	5.5	84

447	The calculation of thermodynamic properties of molecules. *Chemical Society Reviews*, **2010**, 39, 1764-79	58.5	79
446	Computer-Aided Methods and Tools for Chemical Product Design. *Chemical Engineering Research and Design*, **2004**, 82, 1494-1504	5.5	79
445	A model-based systems approach to pharmaceutical product-process design and analysis. *Chemical Engineering Science*, **2010**, 65, 5757-5769	4.4	76
444	Integration of life cycle assessment software with tools for economic and sustainability analyses and process simulation for sustainable process design. *Journal of Cleaner Production*, **2014**, 71, 98-109	10.3	75
443	Selection of Prediction Methods for Thermophysical Properties for Process Modeling and Product Design of Biodiesel Manufacturing. *Industrial & Engineering Chemistry Research*, **2011**, 50, 6809-6836	3.9	75
442	The interactions of design control and operability in reactive distillation systems. *Computers and Chemical Engineering*, **2002**, 26, 735-746	4	75
441	Ionic Liquid Design and Process Simulation for Decarbonization of Shale Gas. *Industrial & Engineering Chemistry Research*, **2016**, 55, 5931-5944	3.9	75
440	A computer-aided software-tool for sustainable process synthesis-intensification. *Computers and Chemical Engineering*, **2017**, 105, 74-95	4	73
439	Techno-economic evaluation of different CO2-based processes for dimethyl carbonate production. *Chemical Engineering Research and Design*, **2015**, 93, 496-510	5.5	73
438	Prediction of heat capacities and heats of vaporization of organic liquids by group contribution methods. *Fluid Phase Equilibria*, **2009**, 283, 49-55	2.5	73
437	Reactive separation systems□ Computation of physical and chemical equilibrium. *Chemical Engineering Science*, **1997**, 52, 527-543	4.4	73
436	Combined Group-Contribution and Atom Connectivity Index-Based Methods for Estimation of Surface Tension and Viscosity. *Industrial & Engineering Chemistry Research*, **2008**, 47, 7940-7954	3.9	71
435	Design and synthesis of distillation systems using a driving-force-based approach. *Chemical Engineering and Processing: Process Intensification*, **2004**, 43, 251-262	3.7	70
434	New Vistas in Chemical Product and Process Design. *Annual Review of Chemical and Biomolecular Engineering*, **2016**, 7, 557-82	8.9	70
433	Integrated business and engineering framework for synthesis and design of enterprise-wide processing networks. *Computers and Chemical Engineering*, **2012**, 38, 213-223	4	68
432	Group-Contribution-Based Estimation of Octanol/Water Partition Coefficient and Aqueous Solubility. *Industrial & Engineering Chemistry Research*, **2002**, 41, 6623-6633	3.9	68
431	Automatic Creation of Missing Groups through Connectivity Index for Pure-Component Property Prediction. *Industrial & Engineering Chemistry Research*, **2005**, 44, 7262-7269	3.9	67
430	Model-based computer-aided framework for design of process monitoring and analysis systems. *Computers and Chemical Engineering*, **2009**, 33, 22-42	4	66

429	Simple new algorithm for distillation column design. *AICHE Journal*, **2000**, 46, 1271-1274	3.6	66
428	Model-Based Calculation of Solid Solubility for Solvent Selection?A Review. *Industrial & Engineering Chemistry Research*, **2008**, 47, 5234-5242	3.9	65
427	Thermal pretreatment of the solid fraction of manure: impact on the biogas reactor performance and microbial community. *Water Science and Technology*, **2006**, 53, 59-67	2.2	65
426	Integration of process design and controller design for chemical processes using model-based methodology. *Computers and Chemical Engineering*, **2010**, 34, 683-699	4	63
425	Ionic liquids for absorption and separation of gases: An extensive database and a systematic screening method. *AICHE Journal*, **2017**, 63, 1353-1367	3.6	62
424	Estimation of the Enthalpy of Vaporization and the Entropy of Vaporization for Pure Organic Compounds at 298.15 K and at Normal Boiling Temperature by a Group Contribution Method. *Industrial & Engineering Chemistry Research*, **2005**, 44, 8436-8454	3.9	62
423	A comprehensive framework for surfactant selection and design for emulsion based chemical product design. *Fluid Phase Equilibria*, **2014**, 362, 288-299	2.5	60
422	Optimal processing pathway for the production of biodiesel from microalgal biomass: A superstructure based approach. *Computers and Chemical Engineering*, **2013**, 58, 305-314	4	60
421	Product design Molecules, devices, functional products, and formulated products. *Computers and Chemical Engineering*, **2015**, 81, 70-79	4	59
420	Process synthesis, design and analysis using a process-group contribution method. *Computers and Chemical Engineering*, **2015**, 81, 245-259	4	56
419	A systematic methodology for design of tailor-made blended products. *Computers and Chemical Engineering*, **2014**, 66, 201-213	4	56
418	Active pharmaceutical ingredient (API) production involving continuous processes--a process system engineering (PSE)-assisted design framework. *European Journal of Pharmaceutics and Biopharmaceutics*, **2012**, 82, 437-56	5.7	55
417	Solvents in organic synthesis: Replacement and multi-step reaction systems. *Computers and Chemical Engineering*, **2008**, 32, 2420-2444	4	55
416	Applications of process synthesis: Moving from conventional chemical processes towards biorefinery processes. *Computers and Chemical Engineering*, **2013**, 49, 217-229	4	54
415	Generic mathematical programming formulation and solution for computer-aided molecular design. *Computers and Chemical Engineering*, **2015**, 78, 79-84	4	53
414	Group contribution based process flowsheet synthesis, design and modelling. *Fluid Phase Equilibria*, **2005**, 228-229, 141-146	2.5	48
413	A grand model for chemical product design. *Computers and Chemical Engineering*, **2016**, 91, 15-27	4	47
412	Estimation of Mixture Properties from First- and Second-Order Group Contributions with the UNIFAC Model. *Industrial & Engineering Chemistry Research*, **2002**, 41, 3260-3273	3.9	46

411	Modeling, simulation and optimization of membrane-based gas separation systems. *Chemical Engineering Science*, **1999**, 54, 943-955	4.4	45
410	A machine learning based computer-aided molecular design/screening methodology for fragrance molecules. *Computers and Chemical Engineering*, **2018**, 115, 295-308	4	44
409	A process synthesis-intensification framework for the development of sustainable membrane-based operations. *Chemical Engineering and Processing: Process Intensification*, **2014**, 86, 173-195	3.7	44
408	Simulation and optimization of fractional crystallization processes. *Chemical Engineering Science*, **1998**, 53, 1551-1564	4.4	44
407	The CAPEC Database*Journal of Chemical & Engineering Data*, **2001**, 46, 1041-1044	2.8	43
406	A multi-layered view of chemical and biochemical engineering. *Chemical Engineering Research and Design*, **2020**, 155, A133-A145	5.5	43
405	Design of formulated products: Experimental component. *AICHE Journal*, **2012**, 58, 173-189	3.6	42
404	Modeling and analysis of vacuum membrane distillation for the recovery of volatile aroma compounds from black currant juice. *Journal of Membrane Science*, **2008**, 320, 442-455	9.6	42
403	Molecular structure based estimation of properties for process design. *Fluid Phase Equilibria*, **1996**, 116, 75-86	2.5	42
402	Prediction of vapor pressure and heats of vaporization of edible oil/fat compounds by group contribution. *Fluid Phase Equilibria*, **2013**, 337, 53-59	2.5	41
401	Graphical and stage-to-stage methods for reactive distillation column design. *AICHE Journal*, **2003**, 49, 2822-2841	3.6	41
400	Systematic integrated process design and control of binary element reactive distillation processes. *AICHE Journal*, **2016**, 62, 3137-3154	3.6	40
399	Application of COSMO-RS and UNIFAC for ionic liquids based gas separation. *Chemical Engineering Science*, **2018**, 192, 816-828	4.4	40
398	Thermodynamic Property Modeling for Chemical Process and Product Engineering: Some Perspectives. *Industrial & Engineering Chemistry Research*, **2009**, 48, 4619-4637	3.9	40
397	Blanket Wash Solvent Blend Design Using Interval Analysis. *Industrial & Engineering Chemistry Research*, **2003**, 42, 516-527	3.9	40
396	OptCAMD: An optimization-based framework and tool for molecular and mixture product design. *Computers and Chemical Engineering*, **2019**, 124, 285-301	4	40
395	A robust methodology for kinetic model parameter estimation for biocatalytic reactions. *Biotechnology Progress*, **2012**, 28, 1186-96	2.8	39
394	Optimal Solvent Design for Extractive Distillation Processes: A Multiobjective Optimization-Based Hierarchical Framework. *Industrial & Engineering Chemistry Research*, **2019**, 58, 5777-5786	3.9	38

393	Chameleonic behavior of ionic liquids and its impact on the estimation of solubility parameters. *Journal of Physical Chemistry B*, **2011**, 115, 12879-88	3.4	38
392	ICAS-PAT: A software for design, analysis and validation of PAT systems. *Computers and Chemical Engineering*, **2010**, 34, 1108-1136	4	38
391	Integration of thermodynamic insights and MINLP optimization for the synthesis, design and analysis of process flowsheets. *Computers and Chemical Engineering*, **2001**, 25, 73-83	4	38
390	Process systems engineering The generation next?. *Computers and Chemical Engineering*, **2021**, 147, 107252	4	38
389	Sustainable chemical processing and energy-carbon dioxide management: Review of challenges and opportunities. *Chemical Engineering Research and Design*, **2018**, 131, 440-464	5.5	37
388	Process systems engineering issues and applications towards reducing carbon dioxide emissions through conversion technologies. *Chemical Engineering Research and Design*, **2016**, 116, 27-47	5.5	37
387	A systematic framework for enterprise-wide optimization: Synthesis and design of processing networks under uncertainty. *Computers and Chemical Engineering*, **2013**, 59, 47-62	4	37
386	A systematic synthesis and design methodology to achieve process intensification in (bio) chemical processes. *Computers and Chemical Engineering*, **2012**, 36, 189-207	4	37
385	Simulation, design, and analysis of azeotropic distillation operations. *Industrial & Engineering Chemistry Research*, **1993**, 32, 620-633	3.9	37
384	Systematic network synthesis and design: Problem formulation, superstructure generation, data management and solution. *Computers and Chemical Engineering*, **2015**, 72, 68-86	4	36
383	Computer aided chemical product design ProCAPD and tailor-made blended products. *Computers and Chemical Engineering*, **2018**, 116, 37-55	4	36
382	A general model for membrane-based separation processes. *Computers and Chemical Engineering*, **2009**, 33, 644-659	4	36
381	Deep learning and knowledge-based methods for computer-aided molecular design oward a unified approach: State-of-the-art and future directions. *Computers and Chemical Engineering*, **2020**, 141, 107005	4	35
380	Are safe results obtained when SAFT equations are applied to ordinary chemicals? Part 2: Study of solid quid equilibria in binary systems. *Fluid Phase Equilibria*, **2012**, 318, 61-76	2.5	35
379	An ontological knowledge-based system for the selection of process monitoring and analysis tools. *Computers and Chemical Engineering*, **2010**, 34, 1137-1154	4	35
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377	Screening for profitable retrofit options of chemical processes: A new method. *AICHE Journal*, **2003** , 49, 2400-2418	3.6	35
376	Multiplicity in numerical solution of non-linear models: Separation processes. *Computers and Chemical Engineering*, **1994**, 18, S55-S61	4	35

375	Chemical product design recent advances and perspectives. *Current Opinion in Chemical Engineering*, **2020**, 27, 22-34	5.4	35
374	Group contribution-based property estimation methods: advances and perspectives. *Current Opinion in Chemical Engineering*, **2019**, 23, 184-196	5.4	34
373	A methodological framework for the development of feasible CO 2 conversion processes. *International Journal of Greenhouse Gas Control*, **2016**, 47, 250-265	4.2	34
372	A method to estimate the enthalpy of formation of organic compounds with chemical accuracy. *Fluid Phase Equilibria*, **2013**, 348, 23-32	2.5	34
371	Properties and CAPE: from present uses to future challenges. *Computers and Chemical Engineering*, **2001**, 25, 3-14	4	34
370	Systematic integrated process design and control of reactive distillation processes involving multi-elements. *Chemical Engineering Research and Design*, **2016**, 115, 348-364	5.5	34
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367	Modeling of the Critical Micelle Concentration (CMC) of Nonionic Surfactants with an Extended Group-Contribution Method. *Industrial & Engineering Chemistry Research*, **2013**, 52, 12236-12246	3.9	32
366	Prediction of acid dissociation constants of organic compounds using group contribution methods. *Chemical Engineering Science*, **2018**, 183, 95-105	4.4	31
365	Integration of design and control through model analysis. *Computers and Chemical Engineering*, **2002**, 26, 213-225	4	31
364	Integration of the biorefinery concept for the development of sustainable processes for pulp and paper industry. *Computers and Chemical Engineering*, **2018**, 119, 70-84	4	31
363	Molecular structure-based methods of property prediction in application to lipids: A review and refinement. *Fluid Phase Equilibria*, **2013**, 357, 2-18	2.5	30
362	A model-based methodology for simultaneous design and control of a bioethanol production process. *Computers and Chemical Engineering*, **2010**, 34, 2043-2061	4	30
361	Systematic Selection of Green Solvents for Organic Reacting Systems. *Chinese Journal of Chemical Engineering*, **2008**, 16, 376-383	3.2	30
360	Estimation of physical properties of amino acids by group-contribution method. *Chemical Engineering Science*, **2018**, 175, 148-161	4.4	28
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356	Solvent selection methodology for pharmaceutical processes: Solvent swap. *Chemical Engineering Research and Design*, **2016**, 115, 443-461	5.5	27
355	Integrated ionic liquid and process design involving azeotropic separation processes. *Chemical Engineering Science*, **2019**, 203, 402-414	4.4	25
354	Computer-aided Framework for Design of Pure, Mixed and Blended Products. *Computer Aided Chemical Engineering*, **2015**, 37, 2093-2098	0.6	25
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348	Computer-aided process intensification: Challenges, trends and opportunities. *AICHE Journal*, **2020**, 66, e16819	3.6	24
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346	Sustainable process design & analysis of hybrid separations. *Computers and Chemical Engineering*, **2017**, 105, 96-104	4	23
345	Computer-aided reaction solvent design based on transition state theory and COSMO-SAC. *Chemical Engineering Science*, **2019**, 202, 300-317	4.4	23
344	Chemical product design: Advances in and proposed directions for research and teaching. *Computers and Chemical Engineering*, **2019**, 126, 147-156	4	23
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342	A combined heuristic and indicator-based methodology for design of sustainable chemical process plants. *Computers and Chemical Engineering*, **2011**, 35, 1343-1358	4	23
341	A Hybrid Modelling Approach for Separation Systems Involving Distillation. *Chemical Engineering Research and Design*, **1999**, 77, 519-534	5.5	23
340	Modelling for dynamic simulation of chemical processes: the index problem. *Chemical Engineering Science*, **1992**, 47, 1311-1315	4.4	23

339	A knowledge based system for the selection of thermodynamic models. *Computers and Chemical Engineering*, **1989**, 13, 397-404	4	23
338	Data, analysis and modeling of physical properties for process design of systems involving lipids. *Fluid Phase Equilibria*, **2014**, 362, 318-327	2.5	22
337	Analysis and prediction of the alpha-function parameters used in cubic equations of state. *Chemical Engineering Science*, **2015**, 126, 584-603	4.4	22
336	Systematic Sustainable Process Design and Analysis of Biodiesel Processes. *Processes*, **2013**, 1, 167-202	2.9	22
335	An experimental verification of morphology of ibuprofen crystals from CAMD designed solvent. *Chemical Engineering Science*, **2007**, 62, 3276-3281	4.4	22
334	Towards the development of a second-order approximation in activity coefficient models based on group contributions. *Fluid Phase Equilibria*, **1996**, 118, 1-12	2.5	22
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326	Analysis of infinite dilution activity coefficients of solutes in hydrocarbons from UNIFAC. *Fluid Phase Equilibria*, **2001**, 181, 163-186	2.5	20
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324	A Computer-Aided Methodology for Mixture-Blend Design. Applications to Tailor-Made Design of Surrogate Fuels. *Industrial & Engineering Chemistry Research*, **2018**, 57, 7008-7020	3.9	19
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316	Determination of optimal energy efficient separation schemes based on driving forces. *Computers and Chemical Engineering*, **2000**, 24, 253-259	4	18
315	A computer aided modeling system. *Computers and Chemical Engineering*, **1999**, 23, S673-S678	4	18
314	Comparative Economic Analysis of Physical, Chemical, and Hybrid Absorption Processes for Carbon Capture. *Industrial & Engineering Chemistry Research*, **2020**, 59, 2005-2012	3.9	17
313	Methodology for design and analysis of reactive distillation involving multielement systems. *Chemical Engineering Research and Design*, **2011**, 89, 1295-1307	5.5	17
312	Computer aided design, analysis and experimental investigation of membrane assisted batch reaction–separation systems. *Computers and Chemical Engineering*, **2009**, 33, 551-574	4	17
311	An Efficient Initialization Procedure for Simulation and Optimization of Large Distillation Problems. *Industrial & Engineering Chemistry Research*, **1997**, 36, 4291-4298	3.9	17
310	Polymer property modeling using grid technology for design of structured products. *Fluid Phase Equilibria*, **2007**, 261, 58-63	2.5	17
309	Model-based computer-aided design for controlled release of pesticides. *Computers and Chemical Engineering*, **2005**, 30, 28-41	4	17
308	Property Integration—A New Approach for Simultaneous Solution of Process and Molecular Design Problems. *Computer Aided Chemical Engineering*, **2002**, 79-84	0.6	17
307	Sustainable solutions by integrating process synthesis-intensification. *Computers and Chemical Engineering*, **2019**, 126, 499-519	4	16
306	Computer-aided design of ionic liquids for hybrid process schemes. *Computers and Chemical Engineering*, **2019**, 130, 106556	4	16
305	Optimal Design of Biodiesel Production Process from Waste Cooking Palm Oil. *Procedia Engineering* , **2012**, 42, 1292-1301		16
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301	A modelling tool for different stages of the process life. *Computer Aided Chemical Engineering*, **2003**, 209-249	0.6	16
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