JosÃ© Palomar

List of Publications by Year
in descending order

139 papers	6,174 citations	41323 49 h-index	85498 71 g-index
142 all docs	142 docs citations	142 times ranked	4801 citing authors

#	Article	IF	Citations
1	Design of biogas upgrading processes based on ionic liquids. Chemical Engineering Journal, 2022, 428, 132103.	6.6	34
2	Extractive Distillation with Ionic Liquids To Separate Benzene, Toluene, and Xylene from Pyrolysis Gasoline: Process Design and Techno-Economic Comparison with the Morphylane Process. Industrial & Engineering Chemistry Research, 2022, 61, 2511-2523.	1.8	17
3	Improvement of CO2 capture processes by tailoring the reaction enthalpy of Aprotic Nâ€'Heterocyclic anion-based ionic liquids. Chemical Engineering Journal Advances, 2022, 10, 100291.	2.4	8
4	Aspen plus supported design of pre-combustion CO2 capture processes based on ionic liquids. Separation and Purification Technology, 2022, 290, 120841.	3.9	23
5	Fine-tune simultaneous dearomatization, desulfurization and denitrogenation of liquid fuels with CO2-derived cyclic carbonates. Fuel, 2022, 321, 124005.	3.4	11
6	Design of Ionic Liquids for Fluorinated Gas Absorption: COSMO-RS Selection and Solubility Experiments. Environmental Science & Technology, 2022, 56, 5898-5909.	4.6	23
7	Universal and low energy-demanding platform to produce propylene carbonate from CO2 using hydrophilic ionic liquids. Separation and Purification Technology, 2022, 295, 121273.	3.9	14
8	Design of hydrodechlorination catalysts on the basis of chloromethanes-metallic active sites interactions. Chemical Engineering Journal, 2022, , 136893.	6.6	3
9	Assessment of bio-ionic liquids as promising solvents in industrial separation processes: Computational screening using COSMO-RS method. Fluid Phase Equilibria, 2022, 560, 113495.	1.4	10
10	Integrated carbon capture and utilization based on bifunctional ionic liquids to save energy and emissions. Chemical Engineering Journal, 2022, 446, 137166.	6.6	15
11	Biocarbonates Derived from CO₂ and Terpenes: Molecular Design for Aqueous Mixture Treatment Driven by COSMO-RS. ACS Sustainable Chemistry and Engineering, 2022, 10, 9635-9643.	3.2	2
12	Techno-economic feasibility of ionic liquids-based CO2 chemical capture processes. Chemical Engineering Journal, 2021, 407, 127196.	6.6	51
13	Understanding the CO2 valorization to propylene carbonate catalyzed by 1-butyl-3-methylimidazolium amino acid ionic liquids. Journal of Molecular Liquids, 2021, 324, 114782.	2.3	15
14	Multiscale evaluation of CO2-derived cyclic carbonates to separate hydrocarbons: Drafting new competitive processes. Fuel Processing Technology, 2021, 212, 106639.	3.7	20
15	Process Analysis of Ionic Liquid-Based Blends as H₂S Absorbents: Search for Thermodynamic/Kinetic Synergies. ACS Sustainable Chemistry and Engineering, 2021, 9, 2080-2088.	3.2	15
16	Close-cycle process to produce CO2-derived propylene carbonate based on amino acid catalyst and water. Journal of CO2 Utilization, 2021, 52, 101656.	3.3	12
17	Extending the ability of cyclic carbonates for extracting BTEX to challenging low aromatic content naphtha: the designer solvent role at process scale. Computers and Chemical Engineering, 2021, 154, 107468.	2.0	10
18	Fatty alcohol/water reaction-separation platform to produce propylene carbonate from captured CO2 using a hydrophobic ionic liquid. Separation and Purification Technology, 2021, 275, 119143.	3.9	13

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19	Modelling and simulation of hollow fiber membrane vacuum regeneration for CO2 desorption processes using ionic liquids. Separation and Purification Technology, 2021, 277, 119465.	3.9	9
20	Thermodynamic and kinetic evaluation of ionic liquids + tetraglyme mixtures on CO2 capture. Journal of CO2 Utilization, 2020, 35, 185-193.	3.3	16
21	Cation and anion effect on the biodegradability and toxicity of imidazoliumâ€“ and cholineâ€“based ionic liquids. Chemosphere, 2020, 240, 124947.	4.2	73
22	Assessment of ionic liquids as H2S physical absorbents by thermodynamic and kinetic analysis based on process simulation. Separation and Purification Technology, 2020, 233, 116050.	3.9	37
23	Development of a method to model the mixing energy of solutions using COSMO molecular descriptors linked with a semi-empirical model using a combined ANN-QSPR methodology. Chemical Engineering Science, 2020, 224, 115764.	1.9	7
24	Extraction of guaiacol from hydrocarbons as an alternative for the upgraded bio-oil purification: Experimental and computational thermodynamic study. Fuel, 2020, 280, 118405.	3.4	20
25	Encapsulated Aminoâ€Acidâ€Based Ionic Liquids for CO₂ Capture. European Journal of Inorganic Chemistry, 2020, 2020, 3158-3166.	1.0	19
26	Design and synthesis of alverine-based ionic liquids to improve drug water solubility. New Journal of Chemistry, 2020, 44, 20428-20433.	1.4	6
27	Tribological properties of gold matrix composite coatings with carbon nanocapsules containing ionic liquid lubricants. Materials Letters, 2020, 279, 128501.	1.3	4
28	Prediction of CO2 chemical absorption isotherms for ionic liquid design by DFT/COSMO-RS calculations. Chemical Engineering Journal Advances, 2020, 4, 100038.	2.4	11
29	Process Evaluation of Fluorinated Ionic Liquids as F-Gas Absorbents. Environmental Science & Technology, 2020, 54, 12784-12794.	4.6	28
30	Siloxanes capture by ionic liquids: Solvent selection and process evaluation. Chemical Engineering Journal, 2020, 401, 126078.	6.6	25
31	Process analysis overview of ionic liquids on CO2 chemical capture. Chemical Engineering Journal, 2020, 390, 124509.	6.6	88
32	Dearomatization of pyrolysis gasoline by extractive distillation with 1-ethyl-3-methylimidazolium tricyanomethanide. Fuel Processing Technology, 2019, 195, 106156.	3.7	28
33	CO₂ Capture by Supported Ionic Liquid Phase: Highlighting the Role of the Particle Size. ACS Sustainable Chemistry and Engineering, 2019, 7, 13089-13097.	3.2	24
34	Stripping Columns to Regenerate Ionic Liquids and Selectively Recover Hydrocarbons Avoiding Vacuum Conditions. Industrial & Engineering Chemistry Research, 2019, 58, 20370-20380.	1.8	18
35	Methanol-Promoted Oxidation of Nitrogen Oxide (NO<i>_x</i>) by Encapsulated Ionic Liquids. Environmental Science & Technology, 2019, 53, 11969-11978.	4.6	10
36	Photostability and photocatalytic degradation of ionic liquids in water under solar light. RSC Advances, 2019, 9, 2026-2033.	1.7	18

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37	Using COSMO-RS to design choline chloride pharmaceutical eutectic solvents. Fluid Phase Equilibria, 2019, 497, 71-78.	1.4	64
38	Electrochemical Co-Deposition of Gold and Carbon Nanocapsules from a Colloidal Suspension. Journal of the Electrochemical Society, 2019, 166, D181-D188.	1.3	2
39	Demonstrating the key role of kinetics over thermodynamics in the selection of ionic liquids for CO2 physical absorption. Separation and Purification Technology, 2019, 213, 578-586.	3.9	59
40	Encapsulation of Ionic Liquids with an Aprotic Heterocyclic Anion (AHA-IL) for CO₂ Capture: Preserving the Favorable Thermodynamics and Enhancing the Kinetics of Absorption. Journal of Physical Chemistry B, 2018, 122, 2616-2626.	1.2	50
41	Molecular and Thermodynamic Properties of Zwitterions versus Ionic Liquids: A Comprehensive Computational Analysis to Develop Advanced Separation Processes. ChemPhysChem, 2018, 19, 794-794.	1.0	4
42	Absorption refrigeration cycles based on ionic liquids: Refrigerant/absorbent selection by thermodynamic and process analysis. Applied Energy, 2018, 213, 179-194.	5.1	88
43	Molecular and Thermodynamic Properties of Zwitterions versus Ionic Liquids: A Comprehensive Computational Analysis to Develop Advanced Separation Processes. ChemPhysChem, 2018, 19, 801-815.	1.0	10
44	Enterprise Ionic Liquids Database (ILUAM) for Use in Aspen ONE Programs Suite with COSMO-Based Property Methods. Industrial & Engineering Chemistry Research, 2018, 57, 980-989.	1.8	71
45	Acetylene absorption by ionic liquids: A multiscale analysis based on molecular and process simulation. Separation and Purification Technology, 2018, 204, 38-48.	3.9	22
46	Novel Process to Reduce Benzene, Thiophene, and Pyrrole in Gasoline Based on [4bmpy][TCM] Ionic Liquid. Energy & Fuels, 2018, 32, 5650-5658.	2.5	15
47	Valorization of chloromethanes by hydrodechlorination with metallic catalysts. Catalysis Today, 2018, 310, 75-85.	2.2	21
48	COSMO-based/Aspen Plus process simulation of the aromatic extraction from pyrolysis gasoline using the {[4empy][NTf 2] + [emim][DCA]} ionic liquid mixture. Separation and Purification Technology, 2018, 190, 211-227.	3.9	67
49	On the volatility of aromatic hydrocarbons in ionic liquids: Vapor-liquid equilibrium measurements and theoretical analysis. Journal of Molecular Liquids, 2018, 250, 9-18.	2.3	13
50	Solubility of carbon dioxide in encapsulated ionic liquids. Separation and Purification Technology, 2018, 196, 41-46.	3.9	31
51	Encapsulated Ionic Liquids to Enable the Practical Application of Amino Acid-Based Ionic Liquids in CO₂ Capture. ACS Sustainable Chemistry and Engineering, 2018, 6, 14178-14187.	3.2	56
52	CO2 conversion to cyclic carbonates catalyzed by ionic liquids with aprotic heterocyclic anions: DFT calculations and operando FTIR analysis. Journal of CO2 Utilization, 2018, 28, 66-72.	3.3	30
53	Assessment the ecotoxicity and inhibition of imidazolium ionic liquids by respiration inhibition assays. Ecotoxicology and Environmental Safety, 2018, 162, 29-34.	2.9	31
54	From kinetics to equilibrium control in CO2 capture columns using Encapsulated Ionic Liquids (ENILs). Chemical Engineering Journal, 2018, 348, 661-668.	6.6	46

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55	Aspen Plus supported analysis of the post-combustion CO2 capture by chemical absorption using the [P2228][CNPyr] and [P66614][CNPyr]AHA Ionic Liquids. International Journal of Greenhouse Gas Control, 2018, 78, 94-102.	2.3	38
56	Deepening of the Role of Cation Substituents on the Extractive Ability of Pyridinium Ionic Liquids of N-Compounds from Fuels. ACS Sustainable Chemistry and Engineering, 2017, 5, 2015-2025.	3.2	22
57	Ionic liquids for post-combustion CO 2 capture by physical absorption: Thermodynamic, kinetic and process analysis. International Journal of Greenhouse Gas Control, 2017, 61, 61-70.	2.3	103
58	Metal-surfactant interaction as a tool to control the catalytic selectivity of Pd catalysts. Applied Catalysis A: General, 2017, 529, 32-39.	2.2	9
59	Hollow Nitrogen- or Boron-Doped Carbon Submicrospheres with a Porous Shell: Preparation and Application as Supports for Hydrodechlorination Catalysts. Industrial & Engineering Chemistry Research, 2017, 56, 7665-7674.	1.8	19
60	Fixed-bed adsorption of ionic liquids onto activated carbon from aqueous phase. Journal of Environmental Chemical Engineering, 2017, 5, 5347-5351.	3.3	26
61	Non-ideal behavior of ionic liquid mixtures to enhance CO2 capture. Fluid Phase Equilibria, 2017, 450, 175-183.	1.4	36
62	Selective Reduction of Nitrite to Nitrogen with Carbon-Supported Pdâ€“AOT Nanoparticles. Industrial & Engineering Chemistry Research, 2017, 56, 11745-11754.	1.8	11
63	Ionic liquids as entrainers for the separation of aromaticâ€“aliphatic hydrocarbon mixtures by extractive distillation. Chemical Engineering Research and Design, 2016, 115, 382-393.	2.7	62
64	Encapsulated Ionic Liquids for CO₂ Capture: Using 1â€Butylâ€methylimidazolium Acetate for Quick and Reversible CO₂ Chemical Absorption.. ChemPhysChem, 2016, 17, 3891-3899.	1.0	51
65	Dechlorination of Dichloromethane by Hydrotreatment with Bimetallic Pd-Pt/C Catalyst. Catalysis Letters, 2016, 146, 2614-2621.	1.4	13
66	Ammonia capture from the gas phase by encapsulated ionic liquids (ENILs). RSC Advances, 2016, 6, 61650-61660.	1.7	45
67	Dicyanamide-based ionic liquids in the liquidâ€“liquid extraction of aromatics from alkanes: Experimental evaluation and computational predictions. Chemical Engineering Research and Design, 2016, 109, 561-572.	2.7	47
68	Aspen Plus supported conceptual design of the aromaticâ€“aliphatic separation from low aromatic content naphtha using 4-methyl-N-butylpyridinium tetrafluoroborate ionic liquid. Fuel Processing Technology, 2016, 146, 29-38.	3.7	67
69	Description of the Behavior of Dichloroalkanes-Containing Solutions with Three [bXmpy][BF4] Isomers, Using the Experimental Information of Thermodynamic Properties, 1H NMR Spectral and the COSMO-RS-Methodology. Journal of Physical Chemistry B, 2015, 119, 3527-3534.	1.2	0
70	Conceptual design of unit operations to separate aromatic hydrocarbons from naphtha using ionic liquids. COSMO-based process simulations with multi-component â€œrealâ€•mixture feed. Chemical Engineering Research and Design, 2015, 94, 632-647.	2.7	58
71	A Comprehensive Comparison of the IEFPCM and SS(V)PE Continuum Solvation Methods with the COSMO Approach. Journal of Chemical Theory and Computation, 2015, 11, 4220-4225.	2.3	274
72	Deactivation behavior of Pd/C and Pt/C catalysts in the gas-phase hydrodechlorination of chloromethanes: Structureâ€“reactivity relationship. Applied Catalysis B: Environmental, 2015, 162, 532-543.	10.8	40

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73	Evaluation of ionic liquids as absorbents for ammonia absorption refrigeration cycles using COSMO-based process simulations. Applied Energy, 2014, 123, 281-291.	5.1	94
74	High Solubilities for Methane, Ethane, Ethylene, and Propane in Trimethyloctylphosphonium Bis(2,4,4-trimethylpentyl) Phosphinate ([P8111][TMPP]). Industrial & Engineering Chemistry Research, 2014, 53, 363-368.	1.8	26
75	Ionic Liquid Mixturesâ€"An Analysis of Their Mutual Miscibility. Journal of Physical Chemistry B, 2014, 118, 2442-2450.	1.2	38
76	Solubility and Diffusivity of CO₂ in [hxmim][NTf₂], [omim][NTf₂], and [dcmim][NTf₂] at <i>T</i> = (298.15, 308.15, and 323.15) K and Pressures up to 20 bar. Journal of Chemical & Engineering Data, 2014, 59, 212-217.	1.0	45
77	Statistical Refinement and Fitting of Experimental Viscosity-to-Temperature Data in Ionic Liquids. Industrial & Engineering Chemistry Research, 2014, 53, 10475-10484.	1.8	23
78	Excess Enthalpy of Monoethanolamine + Ionic Liquid Mixtures: How Good are COSMO-RS Predictions?. Journal of Physical Chemistry B, 2014, 118, 11512-11522.	1.2	82
79	Diffusion Coefficients of CO₂ in Ionic Liquids Estimated by Gravimetry. Industrial & Engineering Chemistry Research, 2014, 53, 13782-13789.	1.8	64
80	Phase behavior of ternary mixtures {aliphatic hydrocarbon+aromatic hydrocarbon+ionic liquid}: Experimental LLE data and their modeling by COSMO-RS. Journal of Chemical Thermodynamics, 2014, 77, 222-229.	1.0	34
81	Enhancing the adsorption of ionic liquids onto activated carbon by the addition of inorganic salts. Chemical Engineering Journal, 2014, 252, 305-310.	6.6	42
82	Experimental data, correlation and prediction of the extraction of benzene from cyclic hydrocarbons using [Epy][ESO4] ionic liquid. Fluid Phase Equilibria, 2014, 361, 83-92.	1.4	19
83	Evaluation of ionic liquids as solvent for aromatic extraction: Experimental, correlation and COSMO-RS predictions. Journal of Chemical Thermodynamics, 2013, 67, 5-12.	1.0	30
84	Screening of RTILs for propane/propylene separation using COSMO-RS methodology. Chemical Engineering Journal, 2013, 220, 284-293.	6.6	65
85	Composition and structural effects on the adsorption of ionic liquids onto activated carbon. Environmental Sciences: Processes and Impacts, 2013, 15, 1752.	1.7	32
86	Selection of Ionic Liquids for Enhancing the Gas Solubility of Volatile Organic Compounds. Journal of Physical Chemistry B, 2013, 117, 296-306.	1.2	75
87	Preparation of hollow submicrocapsules with a mesoporous carbon shell. Carbon, 2013, 59, 430-438.	5.4	21
88	Anion Effects on Kinetics and Thermodynamics of CO₂ Absorption in Ionic Liquids. Journal of Physical Chemistry B, 2013, 117, 3398-3406.	1.2	77
89	Optimized ionic liquids for toluene absorption. AIChE Journal, 2013, 59, 1648-1656.	1.8	90
90	Interactions of Ionic Liquids and Acetone: Thermodynamic Properties, Quantum-Chemical Calculations, and NMR Analysis. Journal of Physical Chemistry B, 2013, 117, 7388-7398.	1.2	68

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91	Adsorption of volatile sulphur compounds onto modified activated carbons: Effect of oxygen functional groups. Journal of Hazardous Materials, 2013, 258-259, 77-83.	6.5	70
92	On the Kinetics of Ionic Liquid Adsorption onto Activated Carbons from Aqueous Solution. Industrial & Engineering Chemistry Research, 2013, 52, 2969-2976.	1.8	32
93	Relation between differential solubility of cellulose and lignin in ionic liquids and activity coefficients. RSC Advances, 2013, 3, 3453.	1.7	58
94	COSMO-RS Studies: Structureâ€“Property Relationships for CO₂ Capture by Reversible Ionic Liquids. Industrial & Engineering Chemistry Research, 2012, 51, 16066-16073.	1.8	65
95	Removal of chlorinated organic volatile compounds by gas phase adsorption with activated carbon. Chemical Engineering Journal, 2012, 211-212, 246-254.	6.6	99
96	Encapsulated ionic liquids (ENILs): from continuous to discrete liquid phase. Chemical Communications, 2012, 48, 10046.	2.2	49
97	Screening ionic liquids as suitable ammonia absorbents on the basis of thermodynamic and kinetic analysis. Separation and Purification Technology, 2012, 95, 188-195.	3.9	73
98	Mechanistic understanding of the behavior of diuron in the adsorption from water onto activated carbon. Chemical Engineering Journal, 2012, 198-199, 346-354.	6.6	27
99	Introducing process simulation in ionic liquids design/selection for separation processes based on operational and economic criteria through the example of their regeneration. Separation and Purification Technology, 2012, 97, 195-204.	3.9	64
100	Developing criteria for the recovery of ionic liquids from aqueous phase by adsorption with activated carbon. Separation and Purification Technology, 2012, 97, 11-19.	3.9	82
101	Comparison of lignin and cellulose solubilities in ionic liquids by COSMO-RS analysis and experimental validation. Industrial Crops and Products, 2012, 37, 155-163.	2.5	105
102	Efficient biodegradation of common ionic liquids by Sphingomonas paucimobilis bacterium. Green Chemistry, 2011, 13, 709.	4.6	66
103	Thermodynamic Behavior of the Binaries 1-Butylpyridinium Tetrafluoroborate with Water and Alkanols: Their Interpretation Using ¹H NMR Spectroscopy and Quantum-Chemistry Calculations. Journal of Physical Chemistry B, 2011, 115, 8763-8774.	1.2	33
104	Understanding the Physical Absorption of CO₂ in Ionic Liquids Using the COSMO-RS Method. Industrial & Engineering Chemistry Research, 2011, 50, 3452-3463.	1.8	174
105	CO₂/N₂ Selectivity Prediction in Supported Ionic Liquid Membranes (SILMs) by COSMO-RS. Industrial & Engineering Chemistry Research, 2011, 50, 5739-5748.	1.8	97
106	Density Functional Theory Analysis of Dichloromethane and Hydrogen Interaction with Pd Clusters: First Step to Simulate Catalytic Hydrodechlorination. Journal of Physical Chemistry C, 2011, 115, 14180-14192.	1.5	41
107	COSMO-RS analysis on mixing properties obtained for the systems 1-butyl-X-methylpyridinium tetrafluoroborate [X = 2,3,4] and 1,Ï‰-dibromoalkanes [Ï‰ = 1â€“6]. Physical Chemistry Chemical Physics, 2011, 13, 7751.	1.3	10
108	Task-specific ionic liquids for efficient ammonia absorption. Separation and Purification Technology, 2011, 82, 43-52.	3.9	140

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109	Characterization of Supported Ionic Liquid Phase (SILP) materials prepared from different supports. Adsorption, 2011, 17, 561-571.	1.4	132
110	A COSMO-RS based guide to analyze/quantify the polarity of ionic liquids and their mixtures with organic cosolvents. Physical Chemistry Chemical Physics, 2010, 12, 1991.	1.3	67
111	A quantum-chemical-based guide to analyze/quantify the cytotoxicity of ionic liquids. Green Chemistry, 2010, 12, 123-134.	4.6	95
112	Thermodynamic study of (alkyl esters+Î±,Ï‰-alkyl dihalides) VII. and for 20 binary mixtures {xCuâˆ'1H2uâˆ'1CO2C3H7+(1âˆ'x)Î±,Ï‰-ClCH2(CH2)vâˆ'2CH2Cl}, where u=1 to 4, Î±=1 and v=Ï‰=2 to 6. An analysis of behavior using the COSMO-RS methodology. Journal of Chemical Thermodynamics, 2009, 41, 367-382.	1.0	2
113	Adsorption of ionic liquids from aqueous effluents by activated carbon. Carbon, 2009, 47, 1846-1856.	5.4	138
114	Development of an a Priori Ionic Liquid Design Tool. 2. Ionic Liquid Selection through the Prediction of COSMO-RS Molecular Descriptor by Inverse Neural Network. Industrial & Engineering Chemistry Research, 2009, 48, 2257-2265.	1.8	60
115	Experimental Thermodynamic Properties of 1-Butyl-2-methylpyridinium Tetrafluoroborate [b2mpy][BF₄] with Water and with Alkan-1-ol and Their Interpretation with the COSMO-RS Methodology. Industrial & Engineering Chemistry Research, 2009, 48, 2678-2690.	1.8	69
116	Effect of Cationic and Anionic Chain Lengths on Volumetric, Transport, and Surface Properties of 1-Alkyl-3-methylimidazolium Alkylsulfate Ionic Liquids at (298.15 and 313.15) K. Journal of Chemical & Engineering Data, 2009, 54, 1297-1301.	1.0	67
117	Modelling of carbon dioxide solubility in ionic liquids at sub and supercritical conditions by neural networks and mathematical regressions. Chemometrics and Intelligent Laboratory Systems, 2008, 93, 149-159.	1.8	41
118	Development of an a Priori Ionic Liquid Design Tool. 1. Integration of a Novel COSMO-RS Molecular Descriptor on Neural Networks. Industrial & Engineering Chemistry Research, 2008, 47, 4523-4532.	1.8	79
119	Prediction of non-ideal behavior of polarity/polarizability scales of solvent mixtures by integration of a novel COSMO-RS molecular descriptor and neural networks. Physical Chemistry Chemical Physics, 2008, 10, 5967.	1.3	20
120	Description of Thermodynamic Behavior of the Systems Formed by Alkyl Ethanoates with 1-Chloroalkanes Using the COSMO-RS Methodology Contributing with New Experimental Information. Industrial & Engineering Chemistry Research, 2008, 47, 3253-3264.	1.8	17
121	Computational Approach to Nuclear Magnetic Resonance in 1-Alkyl-3-methylimidazolium Ionic Liquids. Journal of Physical Chemistry B, 2007, 111, 168-180.	1.2	66
122	Density and Molar Volume Predictions Using COSMO-RS for Ionic Liquids. An Approach to Solvent Design. Industrial & Engineering Chemistry Research, 2007, 46, 6041-6048.	1.8	224
123	Very High Resolution17O NMR Evidence for Displacive Behavior in Hydrogen-Bonded Solids: Squaric Acid. Ferroelectrics, 2004, 302, 23-27.	0.3	3
124	Single-Crystal Magic-Angle Spinning17O NMR and Theoretical Studies of the Antiferroelectric Phase Transition in Squaric Acidâ€. Journal of Physical Chemistry A, 2003, 107, 3471-3475.	1.1	17
125	Quantum Theoretical Evidence for Two Distinct Hydrogen-Bonding Networks and for an Ising Chain Model of the Antiferroelectric Transition in Squaric Acid. Journal of Physical Chemistry B, 2002, 106, 4799-4805.	1.2	10
126	A Density Functional Study of the Complex Nature of the Hydrogen-Bond Network and Mechanism of the Antiferroelectric Transition in Squaric Acid. Ferroelectrics, 2002, 272, 173-179.	0.3	3

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127	Bisquaric Acid:Â Unusual Solid State NMR, Electronic Structure, and a Predicted Orderâˆ'Disorder Transition. Journal of Physical Chemistry A, 2001, 105, 8926-8930.	1.1	9
128	Protonation study of some enamine systems. Computational and Theoretical Chemistry, 2001, 541, 111-117.	1.5	12
129	Theoretical Analysis of Molecular Structure, Hydrogen Bond Strength, and Proton Transfer Energy in Oâˆ'HÂ·Â·O Aromatic Compounds. Journal of Physical Chemistry A, 2000, 104, 6453-6463.	1.1	37
130	Vibrational study of intramolecular hydrogen bonding in o-hydroxybenzoyl compounds. Chemical Physics, 1999, 246, 167-208.	0.9	72
131	Solvatochromism of fluorophores with an intramolecular hydrogen bond and their use as probes in biomolecular cavity sites. International Journal of Quantum Chemistry, 1999, 72, 421-438.	1.0	51
132	The Six-Membered Intramolecular Hydrogen Bond Position as a Switch for Inducing an Excited State Intramolecular Proton Transfer (ESIPT) in Esters ofo-Hydroxynaphthoic Acids. Journal of Physical Chemistry A, 1999, 103, 10921-10934.	1.1	68
133	Gas-phase protolysis between a neutral BrÃ¸nsted acid and a neutral BrÃ¸nsted base?. Chemical Physics Letters, 1998, 293, 511-514.	1.2	15
134	On the acidity and basicity of azoles: the Taft scheme for electrostatic proximity effects. International Journal of Mass Spectrometry and Ion Processes, 1998, 175, 51-59.	1.9	24
135	Intramolecular Proton or Hydrogen-Atom Transfer in the Ground and Excited States of 2-Hydroxybenzoyl Compoundsâ€. Journal of Physical Chemistry A, 1997, 101, 7914-7921.	1.1	110
136	On Solvent Basicity:â€‰ Analysis of the SB Scale. Journal of Physical Chemistry A, 1997, 101, 5183-5189.	1.1	59
137	Double- or single-well potential for GSIPT in 1-hydroxy-2-acetonaphthone?. Chemical Physics Letters, 1997, 269, 151-155.	1.2	32
138	Role of the Structure of Graphene Oxide Sheets on the CO₂ Adsorption Properties of Nanocomposites Based on Graphene Oxide and Polyaniline or Fe₃O₄-Nanoparticles. ACS Sustainable Chemistry and Engineering, 0, , .	3.2	19
139	Process analysis overview of ionic liquids on CO2 chemical capture. , 0, , .		0