Jos Palomar

List of Publications by Year in Descending Order

137 papers	4,711 citations	44 h-index	62 g-index
142 ext. papers	5,414 ext. citations	6 avg, IF	5.85 L-index

#	Paper	IF	Citations
137	Design of biogas upgrading processes based on ionic liquids. *Chemical Engineering Journal*, **2022**, 428, 132103	14.7	10
136	Improvement of CO2 capture processes by tailoring the reaction enthalpy of Aprotic N-Heterocyclic anion-based ionic liquids. *Chemical Engineering Journal Advances*, **2022**, 10, 100291	3.6	2
135	Aspen plus supported design of pre-combustion CO2 capture processes based on ionic liquids. *Separation and Purification Technology*, **2022**, 290, 120841	8.3	3
134	Fine-tune simultaneous dearomatization, desulfurization and denitrogenation of liquid fuels with CO2-derived cyclic carbonates. *Fuel*, **2022**, 321, 124005	7.1	0
133	Universal and low energy-demanding platform to produce propylene carbonate from CO2 using hydrophilic ionic liquids. *Separation and Purification Technology*, **2022**, 121273	8.3	1
132	Design of hydrodechlorination catalysts on the basis of chloromethanes-metallic active sites interactions. *Chemical Engineering Journal*, **2022**, 136893	14.7	
131	Assessment of bio-ionic liquids as promising solvents in industrial separation processes: Computational screening using COSMO-RS method. *Fluid Phase Equilibria*, **2022**, 560, 113495	2.5	0
130	Integrated carbon capture and utilization based on bifunctional ionic liquids to save energy and emissions. *Chemical Engineering Journal*, **2022**, 446, 137166	14.7	0
129	Techno-economic feasibility of ionic liquids-based CO2 chemical capture processes. *Chemical Engineering Journal*, **2021**, 407, 127196	14.7	20
128	Understanding the CO2 valorization to propylene carbonate catalyzed by 1-butyl-3-methylimidazolium amino acid ionic liquids. *Journal of Molecular Liquids*, **2021**, 324, 114782	6	7
127	Multiscale evaluation of CO2-derived cyclic carbonates to separate hydrocarbons: Drafting new competitive processes. *Fuel Processing Technology*, **2021**, 212, 106639	7.2	6
126	Process Analysis of Ionic Liquid-Based Blends as H2S Absorbents: Search for Thermodynamic/Kinetic Synergies. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 2080-2088	8.3	5
125	Close-cycle process to produce CO2-derived propylene carbonate based on amino acid catalyst and water. *Journal of CO2 Utilization*, **2021**, 52, 101656	7.6	4
124	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	4	4
123	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	8.3	2
122	Modelling and simulation of hollow fiber membrane vacuum regeneration for CO2 desorption processes using ionic liquids. *Separation and Purification Technology*, **2021**, 277, 119465	8.3	1
121	Siloxanes capture by ionic liquids: Solvent selection and process evaluation. *Chemical Engineering Journal*, **2020**, 401, 126078	14.7	14

120	Process analysis overview of ionic liquids on CO2 chemical capture. *Chemical Engineering Journal*, **2020**, 390, 124509	14.7	49
119	Assessment of ionic liquids as H2S physical absorbents by thermodynamic and kinetic analysis based on process simulation. *Separation and Purification Technology*, **2020**, 233, 116050	8.3	23
118	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	4.4	4
117	Extraction of guaiacol from hydrocarbons as an alternative for the upgraded bio-oil purification: Experimental and computational thermodynamic study. *Fuel*, **2020**, 280, 118405	7.1	7
116	Encapsulated Amino-Acid-Based Ionic Liquids for CO2 Capture. *European Journal of Inorganic Chemistry*, **2020**, 2020, 3158-3166	2.3	7
115	Design and synthesis of alverine-based ionic liquids to improve drug water solubility. *New Journal of Chemistry*, **2020**, 44, 20428-20433	3.6	3
114	Tribological properties of gold matrix composite coatings with carbon nanocapsules containing ionic liquid lubricants. *Materials Letters*, **2020**, 279, 128501	3.3	1
113	Prediction of CO2 chemical absorption isotherms for ionic liquid design by DFT/COSMO-RS calculations. *Chemical Engineering Journal Advances*, **2020**, 4, 100038	3.6	5
112	Process Evaluation of Fluorinated Ionic Liquids as F-Gas Absorbents. *Environmental Science & Technology*, **2020**, 54, 12784-12794	10.3	11
111	Thermodynamic and kinetic evaluation of ionic liquids + tetraglyme mixtures on CO2 capture. *Journal of CO2 Utilization*, **2020**, 35, 185-193	7.6	10
110	Cation and anion effect on the biodegradability and toxicity of imidazolium- and choline-based ionic liquids. *Chemosphere*, **2020**, 240, 124947	8.4	39
109	Methanol-Promoted Oxidation of Nitrogen Oxide (NO) by Encapsulated Ionic Liquids. *Environmental Science & Technology*, **2019**, 53, 11969-11978	10.3	7
108	Photostability and photocatalytic degradation of ionic liquids in water under solar light. *RSC Advances*, **2019**, 9, 2026-2033	3.7	12
107	Using COSMO-RS to design choline chloride pharmaceutical eutectic solvents. *Fluid Phase Equilibria*, **2019**, 497, 71-78	2.5	33
106	Electrochemical Co-Deposition of Gold and Carbon Nanocapsules from a Colloidal Suspension. *Journal of the Electrochemical Society*, **2019**, 166, D181-D188	3.9	2
105	Dearomatization of pyrolysis gasoline by extractive distillation with 1-ethyl-3-methylimidazolium tricyanomethanide. *Fuel Processing Technology*, **2019**, 195, 106156	7.2	16
104	CO2 Capture by Supported Ionic Liquid Phase: Highlighting the Role of the Particle Size. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 13089-13097	8.3	17
103	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*, **2019**,	8.3	14

102	Stripping Columns to Regenerate Ionic Liquids and Selectively Recover Hydrocarbons Avoiding Vacuum Conditions. *Industrial & Engineering Chemistry Research*, **2019**, 58, 20370-20380	3.9	10
101	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	8.3	36
100	Encapsulation of Ionic Liquids with an Aprotic Heterocyclic Anion (AHA-IL) for CO Capture: Preserving the Favorable Thermodynamics and Enhancing the Kinetics of Absorption. *Journal of Physical Chemistry B*, **2018**, 122, 2616-2626	3.4	38
99	Molecular and Thermodynamic Properties of Zwitterions versus Ionic Liquids: A Comprehensive Computational Analysis to Develop Advanced Separation Processes. *ChemPhysChem*, **2018**, 19, 794-794	3.2	4
98	Absorption refrigeration cycles based on ionic liquids: Refrigerant/absorbent selection by thermodynamic and process analysis. *Applied Energy*, **2018**, 213, 179-194	10.7	61
97	Molecular and Thermodynamic Properties of Zwitterions versus Ionic Liquids: A Comprehensive Computational Analysis to Develop Advanced Separation Processes. *ChemPhysChem*, **2018**, 19, 801-815	3.2	8
96	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	3.9	49
95	Acetylene absorption by ionic liquids: A multiscale analysis based on molecular and process simulation. *Separation and Purification Technology*, **2018**, 204, 38-48	8.3	15
94	Novel Process to Reduce Benzene, Thiophene, and Pyrrole in Gasoline Based on [4bmpy][TCM] Ionic Liquid. *Energy & Fuels*, **2018**, 32, 5650-5658	4.1	10
93	Valorization of chloromethanes by hydrodechlorination with metallic catalysts. *Catalysis Today*, **2018**, 310, 75-85	5.3	14
92	COSMO-based/Aspen Plus process simulation of the aromatic extraction from pyrolysis gasoline using the {[4empy][NTf2] + [emim][DCA]} ionic liquid mixture. *Separation and Purification Technology*, **2018**, 190, 211-227	8.3	45
91	From kinetics to equilibrium control in CO2 capture columns using Encapsulated Ionic Liquids (ENILs). *Chemical Engineering Journal*, **2018**, 348, 661-668	14.7	33
90	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	4.2	26
89	On the volatility of aromatic hydrocarbons in ionic liquids: Vapor-liquid equilibrium measurements and theoretical analysis. *Journal of Molecular Liquids*, **2018**, 250, 9-18	6	9
88	Solubility of carbon dioxide in encapsulated ionic liquids. *Separation and Purification Technology*, **2018**, 196, 41-46	8.3	23
87	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	8.3	42
86	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	7.6	18
85	Assessment the ecotoxicity and inhibition of imidazolium ionic liquids by respiration inhibition assays. *Ecotoxicology and Environmental Safety*, **2018**, 162, 29-34	7	25

84	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	8.3	18
83	Ionic liquids for post-combustion CO2 capture by physical absorption: Thermodynamic, kinetic and process analysis. *International Journal of Greenhouse Gas Control*, **2017**, 61, 61-70	4.2	75
82	Metal-surfactant interaction as a tool to control the catalytic selectivity of Pd catalysts. *Applied Catalysis A: General*, **2017**, 529, 32-39	5.1	7
81	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	3.9	18
80	Fixed-bed adsorption of ionic liquids onto activated carbon from aqueous phase. *Journal of Environmental Chemical Engineering*, **2017**, 5, 5347-5351	6.8	13
79	Non-ideal behavior of ionic liquid mixtures to enhance CO2 capture. *Fluid Phase Equilibria*, **2017**, 450, 175-183	2.5	28
78	Selective Reduction of Nitrite to Nitrogen with Carbon-Supported Pd–AOT Nanoparticles. *Industrial & Engineering Chemistry Research*, **2017**, 56, 11745-11754	3.9	8
77	Ionic Liquids: Bacterial Degradation in Wastewater Treatment Plants **2016**, 1-12		2
76	Encapsulated Ionic Liquids for CO Capture: Using 1-Butyl-methylimidazolium Acetate for Quick and Reversible CO Chemical Absorption. *ChemPhysChem*, **2016**, 17, 3891-3899	3.2	39
75	Dechlorination of Dichloromethane by Hydrotreatment with Bimetallic Pd-Pt/C Catalyst. *Catalysis Letters*, **2016**, 146, 2614-2621	2.8	12
74	Ammonia capture from the gas phase by encapsulated ionic liquids (ENILs). *RSC Advances*, **2016**, 6, 61650-61660	3.9	38
73	Dicyanamide-based ionic liquids in the liquid–liquid extraction of aromatics from alkanes: Experimental evaluation and computational predictions. *Chemical Engineering Research and Design*, **2016**, 109, 561-572	5.5	44
72	Aspen Plus supported conceptual design of the aromatic–aliphatic separation from low aromatic content naphtha using 4-methyl-N-butylpyridinium tetrafluoroborate ionic liquid. *Fuel Processing Technology*, **2016**, 146, 29-38	7.2	54
71	Ionic liquids as entrainers for the separation of aromatic–aliphatic hydrocarbon mixtures by extractive distillation. *Chemical Engineering Research and Design*, **2016**, 115, 382-393	5.5	49
70	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, 4220-5	6.4	155
69	Deactivation behavior of Pd/C and Pt/C catalysts in the gas-phase hydrodechlorination of chloromethanes: Structure–reactivity relationship. *Applied Catalysis B: Environmental*, **2015**, 162, 532-543	21.8	31
68	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, 3527-34	3.4	
67	Conceptual design of unit operations to separate aromatic hydrocarbons from naphtha using ionic liquids. COSMO-based process simulations with multi-component real mixture feed. *Chemical Engineering Research and Design*, **2015**, 94, 632-647	5.5	49

66	Evaluation of ionic liquids as absorbents for ammonia absorption refrigeration cycles using COSMO-based process simulations. *Applied Energy*, **2014**, 123, 281-291	10.7	78
65	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	3.9	22
64	Ionic liquid mixtures--an analysis of their mutual miscibility. *Journal of Physical Chemistry B*, **2014**, 118, 2442-50	3.4	35
63	Solubility and Diffusivity of CO2 in [hxmim][NTf2], [omim][NTf2], and [dcmim][NTf2] at T = (298.15, 308.15, and 323.15) K and Pressures up to 20 bar. *Journal of Chemical & Engineering Data*, **2014** , 59, 212-217	2.8	36
62	Statistical Refinement and Fitting of Experimental Viscosity-to-Temperature Data in Ionic Liquids. *Industrial & Engineering Chemistry Research*, **2014**, 53, 10475-10484	3.9	23
61	Excess enthalpy of monoethanolamine + ionic liquid mixtures: how good are COSMO-RS predictions?. *Journal of Physical Chemistry B*, **2014**, 118, 11512-22	3.4	55
60	Diffusion Coefficients of CO2in Ionic Liquids Estimated by Gravimetry. *Industrial & Engineering Chemistry Research*, **2014**, 53, 13782-13789	3.9	47
59	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	2.9	29
58	Enhancing the adsorption of ionic liquids onto activated carbon by the addition of inorganic salts. *Chemical Engineering Journal*, **2014**, 252, 305-310	14.7	37
57	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	2.5	15
56	Evaluation of ionic liquids as solvent for aromatic extraction: Experimental, correlation and COSMO-RS predictions. *Journal of Chemical Thermodynamics*, **2013**, 67, 5-12	2.9	27
55	Screening of RTILs for propane/propylene separation using COSMO-RS methodology. *Chemical Engineering Journal*, **2013**, 220, 284-293	14.7	52
54	Composition and structural effects on the adsorption of ionic liquids onto activated carbon. *Environmental Sciences: Processes and Impacts*, **2013**, 15, 1752-9	4.3	28
53	Selection of ionic liquids for enhancing the gas solubility of volatile organic compounds. *Journal of Physical Chemistry B*, **2013**, 117, 296-306	3.4	61
52	Preparation of hollow submicrocapsules with a mesoporous carbon shell. *Carbon*, **2013**, 59, 430-438	10.4	18
51	Anion effects on kinetics and thermodynamics of CO2 absorption in ionic liquids. *Journal of Physical Chemistry B*, **2013**, 117, 3398-406	3.4	58
50	Optimized ionic liquids for toluene absorption. *AICHE Journal*, **2013**, 59, 1648-1656	3.6	70
49	Interactions of ionic liquids and acetone: thermodynamic properties, quantum-chemical calculations, and NMR analysis. *Journal of Physical Chemistry B*, **2013**, 117, 7388-98	3.4	61

48	Adsorption of volatile sulphur compounds onto modified activated carbons: effect of oxygen functional groups. *Journal of Hazardous Materials*, **2013**, 258-259, 77-83	12.8	59
47	On the Kinetics of Ionic Liquid Adsorption onto Activated Carbons from Aqueous Solution. *Industrial & Engineering Chemistry Research*, **2013**, 52, 2969-2976	3.9	28
46	Relation between differential solubility of cellulose and lignin in ionic liquids and activity coefficients. *RSC Advances*, **2013**, 3, 3453	3.7	44
45	Comparison of lignin and cellulose solubilities in ionic liquids by COSMO-RS analysis and experimental validation. *Industrial Crops and Products*, **2012**, 37, 155-163	5.9	74
44	COSMO-RS Studies: Structure−Property Relationships for CO2 Capture by Reversible Ionic Liquids. *Industrial & Engineering Chemistry Research*, **2012**, 51, 16066-16073	3.9	57
43	Removal of chlorinated organic volatile compounds by gas phase adsorption with activated carbon. *Chemical Engineering Journal*, **2012**, 211-212, 246-254	14.7	78
42	Encapsulated ionic liquids (ENILs): from continuous to discrete liquid phase. *Chemical Communications*, **2012**, 48, 10046-8	5.8	42
41	Screening ionic liquids as suitable ammonia absorbents on the basis of thermodynamic and kinetic analysis. *Separation and Purification Technology*, **2012**, 95, 188-195	8.3	63
40	Mechanistic understanding of the behavior of diuron in the adsorption from water onto activated carbon. *Chemical Engineering Journal*, **2012**, 198-199, 346-354	14.7	21
39	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	8.3	56
38	Developing criteria for the recovery of ionic liquids from aqueous phase by adsorption with activated carbon. *Separation and Purification Technology*, **2012**, 97, 11-19	8.3	69
37	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	3.8	32
36	COSMO-RS analysis on mixing properties obtained for the systems 1-butyl-X-methylpyridinium tetrafluoroborate [X = 2,3,4] and 1,ω-dibromoalkanes [ω = 1-6]. *Physical Chemistry Chemical Physics*, **2011**, 13, 7751-9	3.6	10
35	Task-specific ionic liquids for efficient ammonia absorption. *Separation and Purification Technology*, **2011**, 82, 43-52	8.3	114
34	Characterization of Supported Ionic Liquid Phase (SILP) materials prepared from different supports. *Adsorption*, **2011**, 17, 561-571	2.6	117
33	Efficient biodegradation of common ionic liquids by Sphingomonas paucimobilis bacterium. *Green Chemistry*, **2011**, 13, 709	10	56
32	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, 8763-74	3.4	31
31	Understanding the Physical Absorption of CO2 in Ionic Liquids Using the COSMO-RS Method. *Industrial & Engineering Chemistry Research*, **2011**, 50, 3452-3463	3.9	148

30	CO2/N2 Selectivity Prediction in Supported Ionic Liquid Membranes (SILMs) by COSMO-RS. *Industrial & Engineering Chemistry Research*, **2011**, 50, 5739-5748	3.9	82
29	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, 1991-2000	3.6	57
28	A quantum-chemical-based guide to analyze/quantify the cytotoxicity of ionic liquids. *Green Chemistry*, **2010**, 12, 123-134	10	75
27	Thermodynamic study of (alkyl esters + alkyl dihalides) VII. HmE and VmE for 20 binary mixtures {xCu H2u CO2C3H7 + (1 x) ClCH2(CH2)v CH2Cl}, where u = 1 to 4, = 1 and v = = 2 to 6. An analysis of behavior using the COSMO-RS methodology. *Journal of Chemical Thermodynamics*, **2009**, 41, 367-382	2.9	2
26	Adsorption of ionic liquids from aqueous effluents by activated carbon. *Carbon*, **2009**, 47, 1846-1856	10.4	125
25	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	3.9	53
24	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	3.9	63
23	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	2.8	64
22	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	3.9	68
21	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, 5967-75	3.6	17
20	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	3.9	17
19	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	3.8	37
18	Computational approach to nuclear magnetic resonance in 1-Alkyl-3-methylimidazolium ionic liquids. *Journal of Physical Chemistry B*, **2007**, 111, 168-80	3.4	65
17	Density and Molar Volume Predictions Using COSMO-RS for Ionic Liquids. An Approach to Solvent Design. *Industrial & Engineering Chemistry Research*, **2007**, 46, 6041-6048	3.9	199
16	Very High Resolution 17O NMR Evidence for Displacive Behavior in Hydrogen-Bonded Solids: Squaric Acid. *Ferroelectrics*, **2004**, 302, 23-27	0.6	3
15	Single-Crystal Magic-Angle Spinning 17O NMR and Theoretical Studies of the Antiferroelectric Phase Transition in Squaric Acid *Journal of Physical Chemistry A*, **2003**, 107, 3471-3475	2.8	16
14	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	3.4	10
13	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	0.6	3

12	Protonation study of some enamine systems. *Computational and Theoretical Chemistry*, **2001**, 541, 111-117		11
11	Bisquaric Acid:Unusual Solid State NMR, Electronic Structure, and a Predicted OrderDisorder Transition. *Journal of Physical Chemistry A*, **2001**, 105, 8926-8930	2.8	8
10	Theoretical Analysis of Molecular Structure, Hydrogen Bond Strength, and Proton Transfer Energy in OHO Aromatic Compounds. *Journal of Physical Chemistry A*, **2000**, 104, 6453-6463	2.8	35
9	Vibrational study of intramolecular hydrogen bonding in o-hydroxybenzoyl compounds. *Chemical Physics*, **1999**, 246, 167-208	2.3	63
8	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	2.1	44
7	The Six-Membered Intramolecular Hydrogen Bond Position as a Switch for Inducing an Excited State Intramolecular Proton Transfer (ESIPT) in Esters of o-Hydroxynaphthoic Acids. *Journal of Physical Chemistry A*, **1999**, 103, 10921-10934	2.8	68
6	Gas-phase protolysis between a neutral Brsted acid and a neutral Brsted base?. *Chemical Physics Letters*, **1998**, 293, 511-514	2.5	13
5	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		19
4	Intramolecular Proton or Hydrogen-Atom Transfer in the Ground and Excited States of 2-Hydroxybenzoyl Compounds *Journal of Physical Chemistry A*, **1997**, 101, 7914-7921	2.8	106
3	On Solvent Basicity: Analysis of the SB Scale. *Journal of Physical Chemistry A*, **1997**, 101, 5183-5189	2.8	52
2	Double- or single-well potential for GSIPT in 1-hydroxy-2-acetonaphthone?. *Chemical Physics Letters* , **1997**, 269, 151-155	2.5	32
1	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*,	3.9	4