In this issue

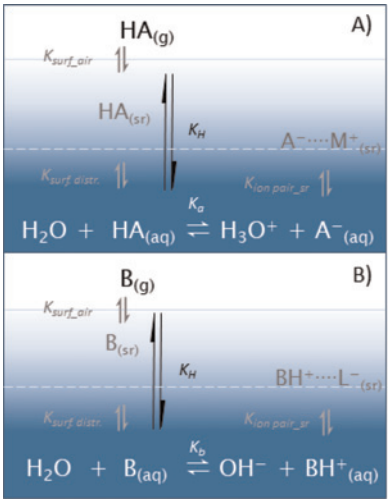
Ingmar Persson, Josephina Werner, Olle Björneholm, Yina Salamanca Blanco, Önder Topel and Éva G. Bajnóczi

Solution chemistry in the surface region of aqueous solutions

https://doi.org/10.1515/pac-2019-1106
Pure Appl. Chem. 2020; 92(10): 1553–1561

Conference paper: The surface region, a number of water molecule layers below the water–air interface, has significantly different physico–chemical properties than bulk water and is involved in a number of equilibria controlling the transport of chemicals between the aqueous bulk and air.

Keywords: aqueous surfaces; chemical equilibrium; chemical speciation; ICSC-36; solution chemistry; XPS.



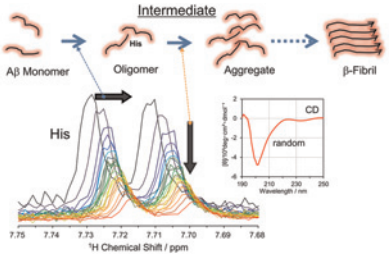
Emiko Okamura and Kenzo Aki

Real-time in-situ ^{1}H NMR of reactions in peptide solution: preaggregation of amyloid-β fragments prior to fibril formation

https://doi.org/10.1515/pac-2019-1201
Pure Appl. Chem. 2020; 92(10): 1575–1583

Conference paper: Real-time NMR detected progress of conversion from amyloid-β monomers to non-structured oligomers and aggregates prior to the fibril formation.

Keywords: Amyloid-β; biological reaction; ICSC-36; oligomers; preaggregation; real-time NMR; spectroscopy.



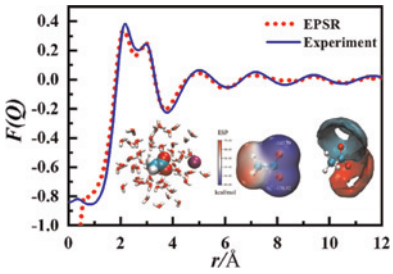
Guangguo Wang, Yongquan Zhou, He Lin, Zhuanfang Jing, Hongyan Liu and Fayan Zhu

Structure of aqueous sodium acetate solutions by X-Ray scattering and density functional theory

https://doi.org/10.1515/pac-2020-0402
Pure Appl. Chem. 2020; 92(10): 1627–1641

Conference paper: X-ray scattering shows that CH3COO⁻ and Na+ mainly exist in the form of SIP, which is consistent with the result from density function theory; and each CH3COO⁻ group binds about 6.23 ± 2.01 to 7.35 ± 1.73 water molecules, suggesting the interaction between CH3COO⁻ and water molecules is relatively strong.

Keywords: density function theory; empirical potential structure refinement; ICSC-36; sodium acetate; solution structure; X-ray scattering.



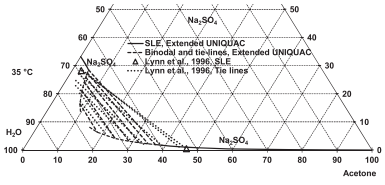
Kaj Thomsen, Martin Due Olsen and Lucas F.F. Corrêa

Modeling vapor-liquid-liquid-solid equilibrium for acetone-water-salt systems

https://doi.org/10.1515/pac-2019-1013
Pure Appl. Chem. 2020; 92(10): 1663–1672

Conference paper: Thermodynamic modeling of acetone-water mixtures with salts.

Keywords: Data compilation; Extended UNIQUAC model; ICSC-36; mixed solvent salt solution.



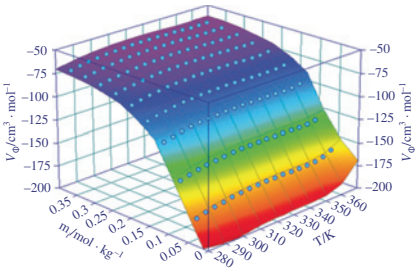
Wanjing Cui, Hongfang Hou, Jiaojiao Chen, Yafei Guo, Lingzong Meng and Tianlong Deng

Apparent molar volumes of sodium arsenate aqueous solution from 283.15 K to 363.15 K at ambient pressure: an experimental and thermodynamic modeling study

https://doi.org/10.1515/pac-2019-1102
Pure Appl. Chem. 2020; 92(10): 1673–1682

Conference paper: The apparent molar volumes, thermal expansion and partial molar volumes were calculated based on the densities of the sodium arsenate aqueous solution, and Pitzer single-salt parameters and temperature-dependence equations were obtained for the first time.

Keywords: apparent molar volume; ICSC-36; Pitzer model; sodium arsenate.



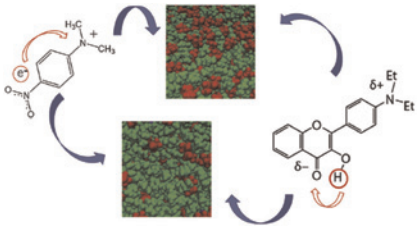
Yoshifumi Kimura

Solvation heterogeneity in ionic liquids as demonstrated by photochemical reactions

https://doi.org/10.1515/pac-2019-1116
Pure Appl. Chem. 2020; 92(10): 1695–1708

Conference paper: Back electron transfer reaction of *N*,*N*-dimethylp-nitroanilne and excited state intramolecular proton transfer reaction of 4′-*N*,*N*-diethylamino-3-hydroxyflavone are investigated in ILs with cations of different alkyl-chain lengths.

Keywords: excitation wavelength dependence; heterogenous structure; ICSC-36; intramolecular electron transfer; intra-molecular proton transfer; ionic liquids.



Éva Böszörményi, Jorge Lado, Csilla Dudás, Bence Kutus, Márton Szabados Gábor Varga, István Pálinkó and Pál Sipos

The structure and composition of solid complexes comprising of Nd(III), Ca(II) and D-gluconate isolated from solutions relevant to radioactive waste disposal

https://doi.org/10.1515/pac-2019-1010
Pure Appl. Chem. 2020; 92(10): 1709–1715

Conference paper:

The structure of the solid complexes $NdGlucH_{-1}(OH) \cdot 2H_2O$ and $CaNdGlucH_{-1}(OH)_3 \cdot 2H_2O$ have been streamlined. Based on the comparison of the diffuse reflectance spectrum of the solids and the molar absorptivity of the solution complexes, the chemical environment of Nd(III) in the solid state is the same as that in the $NdGlucH_{-1}(OH)_0(aq)$ solution species.

Keywords: calcium; D-gluconate; ICSC-36; neodymium; radioactive waste repositories; solid complexes; structure.