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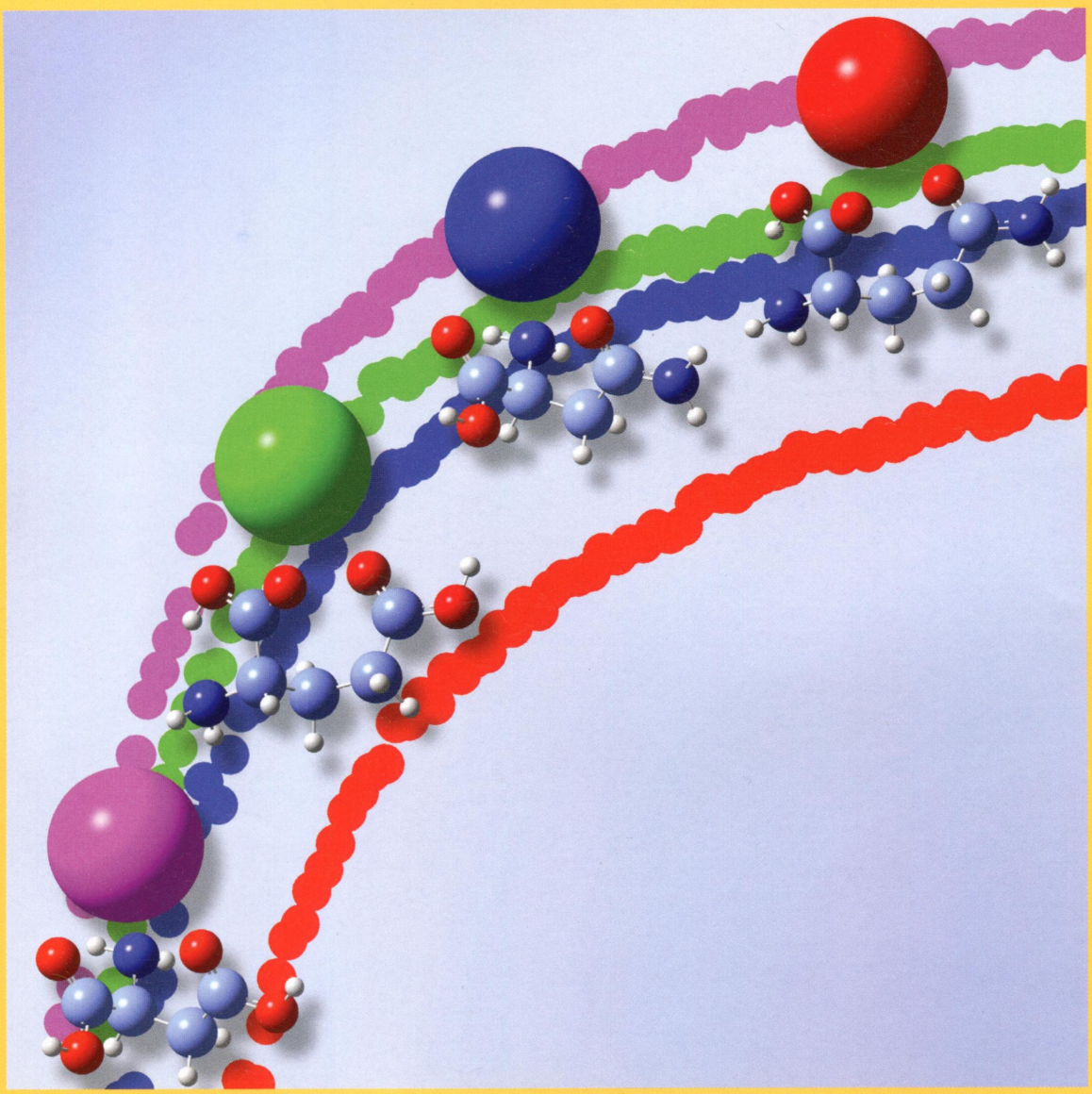

Side-Chain Interactions Enhance the Binding of Alkali Metal Cations to the Acidic Amino Acids and Their Amide Derivatives in the Order: Gln > Asn > Glu > Asp
(see page 5A)

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ON THE COVER: Side-chain interactions enhance the binding of alkali metal cations to the acidic amino acids and their amide derivatives in the order: Gln > Asn > Glu > Asp. Armentrout, Yang, and Rodgers use threshold collision-induced dissociation conducted in a guided ion beam tandem mass spectrometer to measure the bond dissociation energies of rubidium and cesium cations to the acidic amino acids aspartic acid (Asp) and glutamic acid (Glu) and their amide derivatives asparagine (Asn) and glutamine (Gln). In agreement with previous work for complexes analogous to sodium and potassium cations, the order of the quantitative binding energies is Gln > Asn > Glu > Asp (see cover). Variations in these bond energies and those for other amino acids are examined in detail to elucidate trends associated with side-chain functionality and metal cation (inverse with size, $Na^+ > K^+ > Rb^+ > CS^+$). It is shown that the polar side chains of the amide derivatives provide a very good carbonyl binding site that is mediated by the presence of the electron-withdrawing hydroxyl group in the acidic side chains. Longer side chains bind more tightly than shorter side chains, primarily because the polarizability is enhanced. See page 4300.

Articles

Biophysical Chemistry and Biomolecules

4261 dx.doi.org/10.1021/jp408907g
Fragment Orbital Based Description of Charge Transfer in Peptides Including Backbone Orbitals
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4273 (S) dx.doi.org/10.1021/jp410525f
Discovery and Mechanistic Studies of Facile N-Terminal C_α–C Bond Cleavages in the Dissociation of Tyrosine-Containing Peptide Radical Cations
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4282 (S) dx.doi.org/10.1021/jp412140v
Three Stages of Lysozyme Thermal Stabilization by High and Medium Charge Density Anions
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4287 dx.doi.org/10.1021/jp412729r
First Passage Analysis of the Folding of a β-Sheet Miniprotein: Is it More Realistic Than the Standard Equilibrium Approach?
Igor V. Kalgin, Sergei F. Chekmarev,* and Martin Karplus*

4300 (S) dx.doi.org/10.1021/jp5001754
Metal Cation Dependence of Interactions with Amino Acids: Bond Dissociation Energies of Rb^+ and Cs^+ to the Acidic Amino Acids and Their Amide Derivatives
P. B. Armentrout,* Bo Yang, and M. T. Rodgers*

4315 dx.doi.org/10.1021/jp500610t
Preferred Orientations of Phosphoinositides in Bilayers and Their Implications in Protein Recognition Mechanisms
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4326 dx.doi.org/10.1021/jp500795p
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4351 dx.doi.org/10.1021/jp501737x
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4404 dx.doi.org/10.1021/jp4118387

***Structural, Dynamic, and Transport* Properties of Concentrated Aqueous Sodium Chloride Solutions under an External Static Electric Field**
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Toward a pK_a Scale of N-base Amines in Ionic Liquids
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Proton Conduction in Water Ices under an Electric Field
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4425 (S) dx.doi.org/10.1021/jp501207y

Influence of Block Copolymer Compatibilizers on the Morphologies of Semiflexible Polymer/Solvent Blends
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4442 dx.doi.org/10.1021/jp502167t

Favored Composition Design and Atomic Structure Characterization for Ternary Al–Cu–Y Metallic Glasses via Proposed Interatomic Potential
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Additions and Corrections

4450 dx.doi.org/10.1021/jp5031043

Correction to "Theoretical Study of the Hydroxyl Radical Addition to Uracil and Photochemistry of the Formed U6OH• Adduct"
Antonio Francés-Monerris, Manuela Merchán, and Daniel Roca-Sanjuán*

(S) Supporting Information available via online article