In this issue

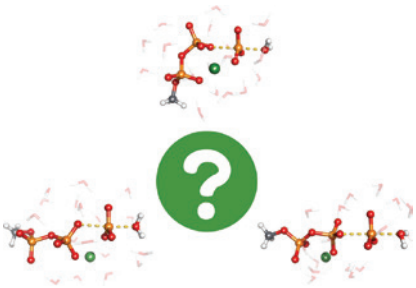
Alexandre Barrozo, David Blaha-Nelson, Nicholas H. Williams and Shina C. L. Kamerlin

The effect of magnesium ions on triphosphate hydrolysis

DOI 10.1515/pac-2016-1125
Pure Appl. Chem. 2017; 89(6): 715–727

Conference paper: How are triphosphates hydrolysed?

Keywords: acetyl phosphate; density functional theory (DFT); ICPOC-23; metals in biology; methyl triphosphate; phosphate hydrolysis.



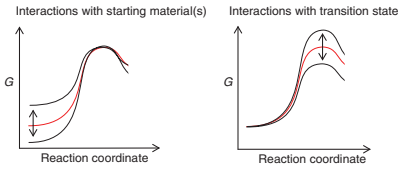
Sinead T. Keaveney, Ronald S. Haines and Jason B. Harper

Ionic liquid solvents: the importance of microscopic interactions in predicting organic reaction outcomes

DOI 10.1515/pac-2016-1008
Pure Appl. Chem. 2017; 89(6): 745–757

Conference paper: Our recent progress on the development of a framework for predicting the effect of an ionic liquid solvent on the outcome of organic processes is summarised. There is a particular focus on the interactions between the ionic liquid and species along the reaction coordinate that have been identified as affecting reaction outcome.

Keywords: activation parameters; ICPOC-23; ionic liquids; organic reactions; rate constants; solvent effects.



Benoit Basdevant, Audrey-Anne Guilbault, Samuel Beaulieu, Antoine Jobin-Des Lauriers and Claude Y. Legault

Iodine(III)-mediated synthesis of chiral α-substituted ketones: recent advances and mechanistic insights

DOI 10.1515/pac-2016-1212
Pure Appl. Chem. 2017; 89(6): 781–789

Conference paper: The iodine(III)-mediated enantioselective synthesis of α-tosyloxy ketones is of synthetic interest, as these products are versatile chiral precursors to access numerous α-chiral ketones. Using joint computational/experimental studies, we have achieved unprecedented levels of selectivities.

Keywords: carbonyl compounds; enols; hypervalent iodine; ICPOC-23; oxidation; reaction mechanisms.

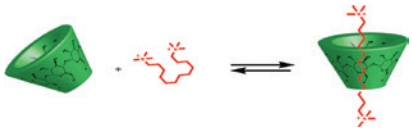
Fernando García-Martínez, Miguel Quiroga, Pedro Rodríguez-Dafonte, Mercedes Parajó and Luis Garcia-Rio

Displacement assay methodology for pseudorotaxane formation in the millisecond time-scale

DOI 10.1515/pac-2016-1101
Pure Appl. Chem. 2017; 89(6): 821–827

Conference paper: Very fast probe displacement (millisecond time-scale) from the host cavity allows kinetic determination of competitive threading/dethreading for pseudorotaxane formation.

Keywords: cyclodextrins; ICPOC-23; kinetics; mechanism; rotaxanes; supramolecular chemistry.



Ofer Reany and N. Gabriel Lemcoff

Light guided chemoselective olefin metathesis reactions

DOI 10.1515/pac-2016-1221
Pure Appl. Chem. 2017; 89(6): 829–840

Conference paper: Orthogonal chemo- and regioselective reactions based on light-activated olefin-metathesis catalysts.

Keywords: chromatic orthogonality; ICPOC-23; latent catalysts; olefin metathesis; photochemistry; ruthenium complexes.