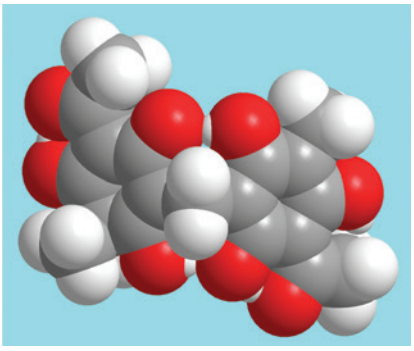
In this issue

Liliana Mammino

Computational study of acylphloroglucinols: an investigation with many branches

https://doi.org/10.1515/pac-2018-0909
Pure Appl. Chem. 2019; 91(4): 597–607

Special topic: Intramolecular hydrogen bonds play the dominant stabilising role in acylphloroglucinol molecules. They are present in all conformers except the very high-energy ones. An intramolecular hydrogen bond between the sp^2 O of the acyl group and a neighbouring OH is present in monomeric acylphloroglucinols. The lower energy conformers of dimeric acylphloroglucinols contain four intramolecular hydrogen bonds, visible in the figure.



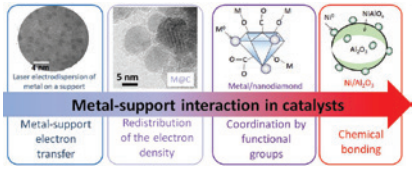
Keywords: acylphloroglucinols; antioxidants; complexes of acylphloroglucinols with a metal ion; Distinguished Women in Chemistry and Chemical Engineering; intramolecular hydrogen bonding; solute-solvent interactions.

Ekaterina S. Lokteva and Elena V. Golubina

Metal-support interactions in the design of heterogeneous catalysts for redox processes

https://doi.org/10.1515/pac-2018-0715
Pure Appl. Chem. 2019; 91(4): 609–631

Special topic: A review of the literature, including the work of the authors, is devoted to the analysis of the interaction of metals with oxide and carbon carriers and its influence on the catalytic properties in redox catalysis reactions. Main attention is paid to metal-support electron transfer, redistribution of electron density, coordination of metal by surface functional groups and by chemical bonding with examples including laser-dispersed metals on a carrier, carbon-capsulated metal and nanodiamond-supported nanoparticles, and Ni/Al_2O_3, correspondingly.



Keywords: carbon support; catalysts; CO oxidation; Distinguished Women in Chemistry and Chemical Engineering; hydrodechlorination; hydrogenation; laser electrodispersion; metal nanoparticles; metal-carbon composite; metal-support interaction; nanodiamond; oxide support.

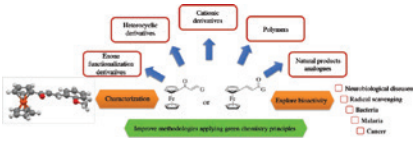
Ingrid Montes-González, Ambar M. Alsina-Sánchez, Juan C. Aponte-Santini, Sara M. Delgado-Rivera and Geraldo L. Durán-Camacho

Perspectives of ferrocenyl chalcones: synthetic scaffolds toward biomedical and materials science applications

https://doi.org/10.1515/pac-2018-0802
Pure Appl. Chem. 2019; 91(4): 653–669

Special topic: Ferrocene and its derivatives constitute versatile and interesting scaffolds with multiple applications that range from biomedical to materials science. This mini-review is focused on ferrocenyl chalcones, emphasizing the methodologies with preeminent yields, and potential applications.

Keywords: aldol reactions; antibiotics; anticancer activity; antimalarial activity; bioactive molecules; bioinorganic chemistry; biomedical applications; Distinguished Women in Chemistry and Chemical Engineering; malaria; materials science; medicinal chemistry; organometallic chemistry; solvent-free reactions.



Natalia P. Tarasova and Alexey A. Zanin

Synthesis of inorganic polymers under ionizing and super high frequency irradiation: role of reaction media

https://doi.org/10.1515/pac-2018-0716
Pure Appl. Chem. 2019; 91(4): 671–686

Special topic:
The article is a generalization of the research of the processes in the phosphorus and sulfur containing systems in the presence of different ionic liquids under γ- and SHF irradiation.

Keywords:
Distinguished Women in Chemistry and Chemical Engineering; elemental phosphorus; elemental sulfur; ionic liquids; ionizing irradiation; reaction media; super high frequency irradiation.