

Special Issue: Coordination Chemistry and Catalysis

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Coordination chemistry plays a key role in the design of functionalized materials, organic and template synthesis, biological systems and catalytic processes. In fact, coordination compounds are deeply related to several types of catalysis. For example, naturally occurring coordination compounds are quite often used as catalytic models, inspiring the design of new synthetic strategies and catalysts. In particular, homogenous catalysis development strongly depends on the suitable design of coordination compounds [1,2].

This Special Issue aimed to cover emerging and promising strategies for the synthesis of new coordination compounds as well as for the development of improved sustainable catalytic chemical transformations by using coordination compounds as catalysts.

The challenging selective oxidation of alcohols to the corresponding carbonyl compounds through sustainable catalytic procedures is addressed by Sutradhar et al. [3] focusing on cleaner synthetic catalytic routes using green oxidants, solvent free processes, energy saving techniques and designing efficient catalysts from environmental and economic perspectives. The synthesis of a mononuclear Cu(II) complex, $[\text{Cu}(\text{kNN}'\text{O-HL})(\text{H}_2\text{O})_2]$, derived from the *N*-acetylpyrazine-2-carbohydrazide (H_2L) ligand and two Fe(III) complexes, $[\text{Fe}(\text{kNN}'\text{O-HL})\text{Cl}_2]$ and $[\text{Fe}(\text{kNN}'\text{O-HL})\text{Cl}(\mu\text{-OMe})_2]$ is presented as well as their application as catalytic precursors for the oxidation of primary and secondary benzyl alcohols (benzyl alcohol, 1-phenyl alcohol) and secondary aliphatic alcohols (cyclohexanol) with *tert*-butyl hydroperoxide (TBHP) as an oxidising agent under solvent-free low power microwave (MW) irradiation. All the catalyst precursors led to very good yields and selectivity towards the oxidation of the tested alcohols. Catalyst regioselectivity and the use of neat systems under low power MW irradiation were significant factors regarding the increase in the sustainability of catalytic synthetic systems.

Another extremely important industrial catalytic reaction is ethylene polymerization, as polyethylene, due to its extensive number of applications, has been playing an imperative role in our daily life and industry. The physical and mechanical properties of polyethylene strongly depend on the structure of the product, which can be adjusted by a transition metal coordination compound (catalyst) during ethylene oligomerization or polymerization. This issue is addressed by Sun et al. [4], focusing on the different variation trend of catalytic activities for two Ni analogue systems using the multiple linear regression analysis (MLRA) method which allows the prediction of the catalytic activities by considering both the electronic (Q_{eff} and Hammett constant F) and steric effects (θ and β). Five electronic and two steric descriptors are selected as the independent variables in linear fitting, including Hammett constants (F), effective net charge (Q_{eff}), energy difference (ΔE), HOMO–LUMO energy gap ($\Delta \epsilon_1$, $\Delta \epsilon_2$), the open cone angle (θ), and bite angle (β). The found contribution of each descriptor indicated that the effective net charge (Q_{eff}) plays the dominant role in order to determine the variation of catalytic activities in one of the Ni systems, while in the other, the open cone angle (θ) becomes the major factor due to the variation of the fused member-ring. Thus, the study clarified the

major factor on catalytic activity of different Ni systems, which is helpful in providing guidance to predict and design new Ni complexes with desirable catalytic properties.

This Special Issue also includes a review paper by Khalimon et al. [5], dealing with the development of efficient methodologies for the production of amines. In this regard, deoxygenative reduction of amides to amines by means of coordination compounds catalysed hydrogenation, hydrosilylation, and hydroboration reactions is an attractive alternative to conventional wasteful techniques based on stoichiometric reductions of amides and imines, or the reductive amination of aldehydes with metal hydride reagents. However, the relatively low electrophilicity of the amide carbonyl group makes this transformation more challenging when compared to reduction of other carbonyl compounds. The review is focused on current achievements in the deoxygenative hydrogenation, hydrosilylation, and hydroboration of amides to amines, paying special attention to the design of metal catalysts and mechanisms of such important catalytic transformations.

Another review paper by Pályi et al. [6], dealing with the synthetic progress on coordinated “naked” pnictogenes and their role on homogeneous molecular catalysis, is also part of this Special Issue. In fact, the type of organometallic complexes bearing diphosphorous (P_2) side-on coordinated to a dinuclear centre induced several ingenious new ramifications in main-group/transition metal cluster chemistry (e.g., in the field of atmospheric N_2 fixation) in the last decades which are highlighted in the review.

As the guest editor of this Special Issue, I am thankful to all the contributors for their interest and valuable support and also to the MDPI staff members for their editorial support. I trust the readers will find the papers of this Special Issue interesting and helpful for the synthesis and design of new coordination compounds and/or their application in catalysis.

Conflicts of Interest: The author declares no conflict of interest.

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