PULSUS
WWW.PULSUSCONFERENCE.COM
35 YEARS IN ASSESSING THE IMPACT OF HEALTHCARE RESEARCH

3rd International conference on

Green Chemistry and Technology

March 14, 2022 | Webinar

Quantitative investigation of the catalytic activities of analogues nickel complexes in ethylene oligo-/polymerization

Arfa Abrar Malik

Institute of Chemistry, Chinese Academy of Sciences, China

Catalytic activity is the most important property among the catalytic performance of transition metal complexes. Many achievements have been obtained previously on increasing the catalytic activity of complex, by the modification of ligands, the change of substitutions on ligands as well as the design of new structure of ligand [1-2]. However, the potential principle of transition metal complex with high catalytic activity is still necessary to be clarified at the molecular level. The catalytic activity is fundamentally determined by the structure of catalyst, including the electronic and steric effects. To expose the relationship between catalyst structure and reaction activity, two carbocyclic fused pyridineimine nickel analogue systems (Ni1 and Ni2) with different fused member ring are investigated [3-4]. Multiple linear regression analysis is performed by means of five electronic and two steric descriptors, including Hammett constant (F), effective net charge (Q_{eff}), energy difference (ΔE), HOMO–LUMO energy gap ($\Delta \varepsilon_1$, $\Delta \varepsilon_2$), open cone angle (θ), and bite angle (β) [5]. The value of correlation coefficient values (R^2) is over 0.938 obtained by using the combinations of effective net charge (Q_{eff}) and open cone angle (θ) for both individual and comparison analogues systems. The contribution analysis indicates that the dominant descriptor is effective net charge (Q_{eff}) in Ni1 system and open cone angle (θ) in Ni2 systems, respectively.
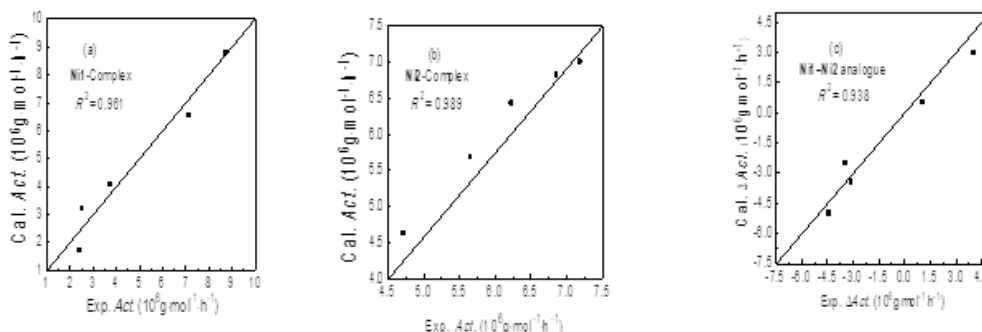

Fig 1. Comparisons between calculated and experimental activities of (a) Ni1 system, (b) Ni2 system, and (c) Ni1–Ni2 analogue system, using the descriptors of effective net charge (Q_{eff}) and open cone angle (θ).

arfamalik@iccas.ac.cn