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

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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. 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. Multiple linear regression analysis is performed by means of five electronic and two steric descriptors, including Hammett constant (F), effective net charge (Qeff), energy difference (ΔE), HOMO–LUMO energy gap (Δε1, Δε2), open cone angle (θ) and bite angle (β). The value of correlation coefficient values (R2) is over 0.938 obtained by using the combinations of effective net charge (Qeff) and open cone angle (θ) for both individual and comparison analogues systems. The contribution analysis indicates that the dominant descriptor is effective net charge (Qeff) in Ni1 system and open cone angle (θ) in Ni2 systems, respectively [Figure 1].

Biography

Arfa Abrar Malik is a PhD research scholar at the Institute of Chemistry, Chinese Academy of Science Beijing China. Her research work is focused on the synthesis of transition metal complexes and the effect of their activities on ethylene polymerization. Her research focus for the duration of her PhD is to synthesize organometallic complexes of Iron and Cobalt and correlate her experimental results with the models/simulations, which she computed during her MS research. She also managed to successfully publish her MS research based on the simulation and models of the transition metal complexes and their enhancement as catalysts in ethylene oligo/polymerization. Currently, she is working as an exchange researcher at the Department of Chemistry, Quaid-i-Azam University Islamabad, Pakistan. Apart from her philanthropic activities, she is Co-Founder at WEmpower Pakistan and also affiliated with this international non-profit organization as the Chief Information Officer and works towards bridging the gap between competent students and academia. She advises students regarding their PhD applications and scholarships.

Received: February 09, 2023; **Accepted**: February 12, 2023; **Published**: February 20, 2023