Toward Next-Generation Plastics: Quantifying the Donor Ability of Schiff Base Ligands for Olefin Polymerization Catalysis

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Polyolefins are typically produced using early transition metal catalysts. While these catalysts produce polymers with a wide variety of properties, they are incompatible with polar monomers. Recently, late transition metal catalysts have attracted attention due to their tolerance of and ability to incorporate polar monomers, which is desirable because of the unique properties they can impart on the resulting polymer, such as compatibility with polar materials, increased adhesion, and biodegradability. However, the synthesis of polar polyolefins remains an unmet challenge in industry due to the limited tunability of catalyst performance. To advance the development of a system for the logical design of polyolefin catalysts, understanding how the electronic properties of ligands influence catalyst reactivity and the properties of the resulting polymer are essential. To investigate this, 195Pt nuclear magnetic resonance (NMR) spectroscopy was used to quantify the donor ability of different ligands based on their 195Pt chemical shift. In this model system, platinum was coordinated with varying Schiff base ligands, resulting in four complexes which were analyzed using 195Pt NMR. We observed that the addition of a methyl group para to the oxygen bound to platinum was electronically distinguishable, whereas the addition of two isopropyl groups ortho to the nitrogen bound to platinum did not change the chemical shift, suggesting that the methyl group is slightly electron withdrawing, and the isopropyls have no electronic effect. These chemical shifts will be compared to catalyst activity to find correlations that would form the basis of a parameterization method for catalyst tunability.

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