Analysis of Catalytic Performance by Machine Learning for Understanding of Ethylene/Methyl Acrylate Copolymerization Catalyzed by Palladium/Phosphine–Sulfonate Complexes

([1]*Graduate School of Engineering, The University of Tokyo*, [2]*Department of Chemistry, The University of Utah*) ○Shumpei Akita,[1] Jing-Yao Guo,[2] Matthew S. Sigman,[2] Kyoko Nozaki,[1]
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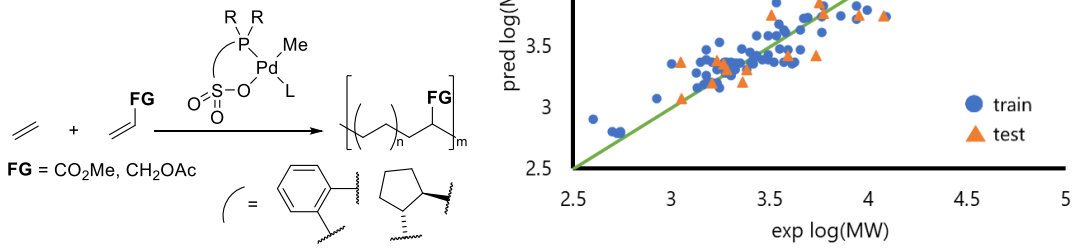
Various types of palladium complexes bearing phosphine-sulfonate ligands have been developed for the coordination–insertion copolymerization of olefins with polar monomers.[1] Characteristic features of the ligands, such as electronic[2] and steric[3] properties were discussed in relation to their catalytic performance: for example, the stronger electron-donation from the phosphine to the metal center[2] and the larger B5 parameter of the substituents on the phosphorus atom,[3] both increased the molecular weight of the obtained polyethylene. Aiming at further analysis of the obtained data for the copolymerization of ethylene and methyl acrylate, we developed prediction methods for molecular weight, catalytic activity, and incorporation of methyl acrylate using machine learning.

The result of prediction for molecular weight of the copolymer is shown below. In the prediction, R^2 and Q^2 are larger than 0.85 and 0.80, respectively, suggesting their good agreement. The important parameters for prediction of molecular weight were clarified to be Sterimol B5 parameter of the substituents on phosphorus atom, %Vbur, and occupancy of d_{z2} orbital in palladium.



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