Predicting Ligand-to-Metal Coordination Modes by a Combination of Coordination Templates and Machine Learning

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Design of novel organometallic complexes for functional materials and applications in homogenous catalysis heavily dependent if a generated ligand is able to coordinate to metals in a correct way. This research article presents a synergistic model for predicting ligand-to-metal coordination modes, which leverages the use of machine-extracted cheminformatics reaction rules to generate possible coordination structures per complex that are further subjected to ranking via directed-message passing neural network.