**Digital Chemistry Guided Development of Novel Ligands for Selective Ethylene Tetramerization**

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**Abstract:** Oligomerization of ethylene to linear alpha olefins is a valuable industrial catalytic process. Conventional non-selective catalysts produce a broad Schulz-Flory distribution of various ethylene oligomers, many of which are low-value. To target on-demand production of valuable 1-octene, highly active homogeneous catalysts based on Cr active sites and supported by diphosphinoamine (PNP) ligands have been known to selectively tetramerize ethylene for nearly two decades. However, deployment of these catalysts is hindered economically by inevitable formation of byproducts including 1-hexene, methylcyclopentane, methylenecyclopentane, and polyethylene, which is especially pernicious as its insolubility requires reactor downtime to remove. To accelerate catalyst discovery, we have developed several digital chemistry strategies to help identify promising PNP variants. (1) PNP ligand solubility is correlated with catalyst activity. (2) Calculated thermodynamic stability of PNP ligand against isomerization to bisphosphinoimine (PPN), calculated via density functional theory (DFT), is correlated with lower PE selectivity. (3) The steric bulk of the ligand, measured via SambVca buried volume calculations, is correlated with various product selectivities. Combining these various digital chemistry guides, we have developed and patented novel PNP ligands with higher catalytic activity, lower PE selectivity, and greater overall linear alpha olefin selectivity.

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