

Selectivity of Cr-catalyzed Ethylene Oligomerization in Confined Geometries

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Abstract: Over the last decade, increased interest in the development of selective ethylene oligomerization catalysts has led to a diverse array of catalytic systems based on chromium.¹ However, tuning the C₆/C₈ selectivity of Cr-catalyzed oligomerization of ethylene still remains a central topic in this area.¹ We have recently demonstrated the concept of confinement-governed olefin-metathesis-based selective macro(mono)cyclization by utilizing catalysts immobilized inside the pores of mesoporous silica.^{3,4} Here, the main aim is to exploit confinement effects to selectively produce trimeric or tetrameric products from ethylene, i.e., 1-hexene or 1-octene, respectively. We use immobilized *N*-heterocyclic carbene and cyclic alkyl aminocarbene Cr-catalysts that are robust and promising alternatives to existing Cr-complexes. We aim to exploit constrained geometries to selectively stabilize transition geometries that lead to the desired end products and we will leverage acidity, polarity and π -donating abilities of the support. Our initial efforts suggest that the silica-supported catalysts are promising to selectively produce lower linear α -olefins (LAOs).

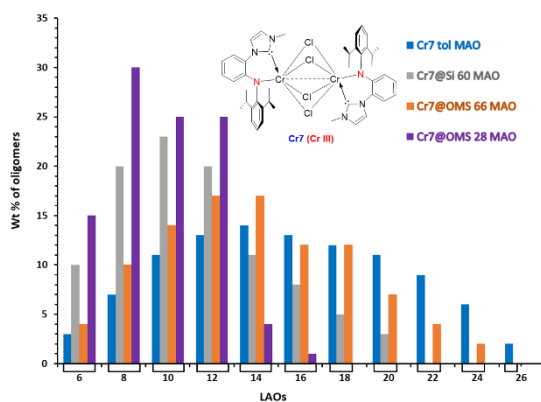


Figure 1: Oligomer distribution with Cr7 catalyst using MAO as cocatalyst.

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[3] F. Ziegler *et al.* *J. Am. Chem. Soc.* 2019, **141**, 19014–19022, 10.1021/jacs.9b08776.
[4] F. Ziegler *et al.* *ACS Catal.* 2021, **11**, 11570–11578, 10.1021/acscatal.1c03057.