**Ethylene Tetramerization: Mechanism and Role of Solvent**

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Chromium diphosphinoamine (PNP) catalysts are among the most successful for ethylene tetramerization to 1-octene, although byproducts such as 1-hexene or polyethylene are inevitably formed. To address this challenge, we have explored the mechanism of ethylene tetramerization catalysts with density functional theory (DFT). The roles of certain solvents on catalyst activity and product selectivity are supported by computational modelling and experimental catalytic testing.