

Molecular active sites in heterogeneous Ir-La/C catalyzed carbonylation of methanol to acetates

곽자훈*
울산과학기술대
(jhwak@unist.ac.kr*)

Homogenous catalysts show manifest selectivity and facilitate mechanistic understanding, but encounter separation and stability problems. Heterogeneous catalysts are more widely used in industry on account of their robustness and separability from product streams, but normally contain a multiplicity of active sites, diminishing selectivity and hindering mechanistic interpretations. Attaining molecular (single site) behavior similar to homogenous catalysis on heterogeneous surfaces has thus been an enduring goal. Here I show that when Ir and La halides are deposited on carbon, exposure to CO spontaneously generates a discrete molecular heterobimetallic structure containing an Ir-La bond, likely $\text{IrLa}(\text{CO})_2\text{Cl}_4$, that acts as a highly active and selective heterogeneous catalyst for the carbonylation of methanol to produce acetic acid. The activity may be mechanistically rationalized based on the chemistry of lanthanide-transition metal complexes.