

Palladium-catalyzed reductive carbonylation of nitrobenzene

느윙 탄 똥, 트란 안 비¹, 이혜진¹, 박소연, 백자연, 김용진[†]

한국생산기술연구원; ¹과학기술연합대학원대학교

(yjkim@kitech.re.kr[†])

Organic isocyanates (R-NCO) have achieved great commercial importance as chemical intermediates in the manufacture of many useful chemicals. However, conventional route has two serious problems: (i) the use of extremely toxic phosgene in the carbonylation step and (ii) the production of a large amount of corrosive hydrochloric acid after reaction. Direct carbonylation with carbon monoxide is an attractive alternative, as it can provide a one-step conversion of nitro aromatics to the corresponding isocyanate without the use of menacing phosgene. In this research, direct reductive carbonylation of nitrobenzene to phenyl isocyanate with carbon monoxide was performed using various types of palladium catalysts together with many types of N-donor ligands. The effect of reaction time, pressure, temperature, ligand amount, and molar ratio was also investigated to establish the optimized conditions. The active catalyst Pd(1-C₄Im)₂Cl₂ was also synthesized and able to achieve comparable result. Furthermore, plausible mechanism was proposed based on spectroscopic and mechanistic studies.