

Ionic Liquids - Catalysts for the Synthesis of Quinazoline-2,4-diones from 2-Aminobenzonitrile and CO₂

M. Hulla¹, S. M. Chamam¹, G. Laurenczy¹, S. Das², P. J. Dyson^{1*}

¹EPFL Lausanne, ²Georg-August-Universität Göttingen

Ionic liquids (ILs) are versatile solvents and catalysts for the synthesis of quinazoline-2,4(1H,3H)-dione from 2-aminobenzonitrile and CO₂. However, the catalytic role of the IL in this reaction is poorly understood. Here, we present a systematic investigation of a series of ILs in this reaction and showed that the IL cation does not play a significant role in the catalytic activation of the substrates. The IL cation only plays a secondary role in contributing to the control of the desired physical properties of the IL. A linear relationship between the pK_a of the IL anion and the reaction rate was identified with maximum catalyst efficiency observed at a pK_a of 14.7 and above in DMSO. The base catalyzed reaction is limited by the acidity of the quinazoline-2,4(1H,3H)-dione product, which is deprotonated by more basic catalysts leading to the formation of the quinazolide anion (conjugate acid pK_a 14.7). Neutralization of the original catalyst and formation of new quinazolide anion catalyst leads to the observed reaction limit. Finally, we demonstrate that ILs containing the quinazolide anion are the most active base catalysts for the synthesis of quinazoline-2,4(1H,3H)-dione from 2-aminobenzonitrile and CO₂.

