

Acetyl nitrate nitrations in [bmpy][N(Tf)₂] and [bmpy][OTf], and the recycling of ionic liquids

Emilie Dal and N. Llewellyn Lancaster*

Department of Chemistry, King's College London, Strand, London, WC2R 2LS, UK; E-mail: llewellyn.lancaster@kcl.ac.uk

Kinetic data

All reactions were performed at 25 °C under a nitrogen atmosphere. Graphs of concentration against time were plotted, and from these, the initial rate of reaction (V_0) was estimated. These data are reported below for the nitration of toluene in dichloromethane where $[\text{Ac}_2\text{O}]_0$ was held constant (table S1) and where $[\text{HNO}_3]_0$ was held constant (table S2).

Likewise, data are reported for the nitration of chlorobenzene in [bmpy][N(Tf)₂] where $[\text{Ac}_2\text{O}]_0$ was held constant (table S3) and where $[\text{HNO}_3]_0$ was held constant (table S4).

By plotting $\log_{10} V_0$ against $\log_{10} [\text{X}]_0$, it is possible to estimate the order of reaction with respect to [X]. This has been done, and is reported in each table.

Table S1 Nitration of toluene in CH₂Cl₂ with varied $[\text{HNO}_3]_0$; $[\text{Ac}_2\text{O}]_0$ ca. 0.84 M.

$[\text{HNO}_3]_0 / \text{M}$	$V_0 / \text{M min}^{-1}$	Approx. order wrt $[\text{HNO}_3]_0$
0.39	0.05	3
0.44	0.06	
0.65	0.25	

Table S2 Nitration of toluene in CH₂Cl₂ with varied $[\text{Ac}_2\text{O}]_0$; $[\text{HNO}_3]_0$ ca. 0.43 M.

$[\text{Ac}_2\text{O}]_0 / \text{M}$	$V_0 / \text{M min}^{-1}$	Approx. order wrt $[\text{Ac}_2\text{O}]_0$
0.56	0.012	3
0.88	0.060	
1.0	0.070	

Table S3 Nitration of chlorobenzene in [bmpy][N(Tf)₂] with varied $[\text{HNO}_3]_0$; $[\text{Ac}_2\text{O}]_0$ ca. 0.82 M.

$[\text{HNO}_3]_0 / \text{M}$	$V_0 / \text{M min}^{-1}$	Approx. order wrt $[\text{HNO}_3]_0$
0.43	0.067	2
0.48	0.083	
0.49	0.083	
0.67	0.17	

Table S4 Nitration of chlorobenzene in [bmpy][N(Tf)₂] with varied [Ac₂O]₀; [HNO₃]₀ *ca.* 0.56 M.

[Ac ₂ O] ₀ / M	<i>V</i> ₀ / M min ⁻¹	Approx. order wrt [Ac ₂ O] ₀
0.67	0.011	
0.74	0.020	5 or higher
1.0	0.10	