Supporting information

A Pathway to Vinyl Chloride Production via Dehydrochlorination of 1,2-Dichloroethane in Ionic Liquid Media

Tom Boudewijns[a], Marco Piccinini[b], Paul Degraeve[b], Armin Liebens[b] and Dirk De Vos*[,a]

[a]Centre for Surface Chemistry and Catalysis, Department Molecular and Microbiological Systems, KU Leuven, 3000 Leuven, Belgium.
[b]Solvay SA, Rue de Ransbeek 310, 1120 Brussels, Belgium.

E-mail: dirk.devos@biw.kuleuven.be

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Experimental section

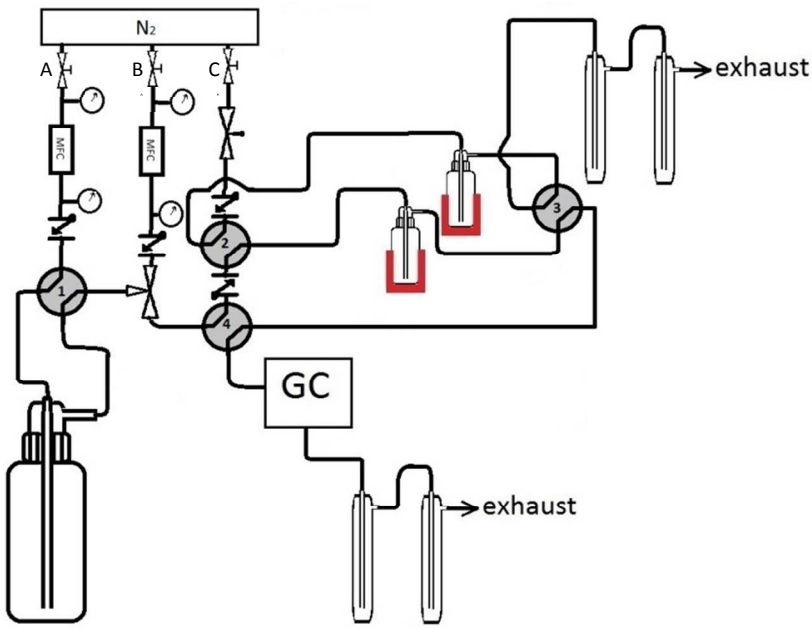

Figure S1: Scheme of the reactor set-up

Experiments were performed in a reactor set-up as depicted in figure S1. This set-up consists of three separate gas lines supplying dry N_2. The first two lines (A and B) are controlled via mass flow controllers (MFC), while the third line (C) is controlled with a needle valve. Via a 4-way cross-over valve **1**, N_2-flow A can either be sent through a saturator at room temperature (typically containing 1,2-DCE) or bypass this saturator. Afterwards the gas flow is diluted with N_2-line B. The resulting gas flow goes via 4-way cross over valve **4** either directly to the GC or to the reactor part. In this part 2 reactors are connected in

parallel; 4-way cross over valve **2** is used to connect to either one of the reactors. 4-way cross over valve **3** controls the outlet of the reactors, which can be sent either to the exhaust or to the GC. At the outlet double washing bottles are installed, of which the second one is filled with water to strip out HCl. The first one is to prevent back-splashing of the water. N_2-line C is used to flush the reactors after reaction.

The reactor is typically filled with 6 mmol of ionic liquid, unless stated otherwise. Prior to loading into the reactor, the ionic liquid is dried using a Schlenk line. The reaction temperature varies between 180 °C and 240 °C, with a stirring rate of 1000 rpm, controlled by a temperature controlled stirring plate. The standard gas flow is 5 ml/min through N_2-line A and 5 ml/min through N_2-line B, resulting in a total gas flow of 10 ml/min containing 5 vol% 1,2-DCE. The reactor effluent was analyzed using a Shimadzu 2010 GC plus equipped with a 25m CP-Porabond PLOT Q column, with inner diameter 0.53 mm and film thickness of 10 µm and an FID detector.

When higher feeding rates were applied, liquid 1,2-DCE was fed to the redesigned reactor (figure S2) by means of a B. Braun Perfusor®Space type 8713030 pump together with a guiding N_2-flow from line A. The reactor effluent was diluted with N_2 from line B to prevent condensation in the transfer lines.

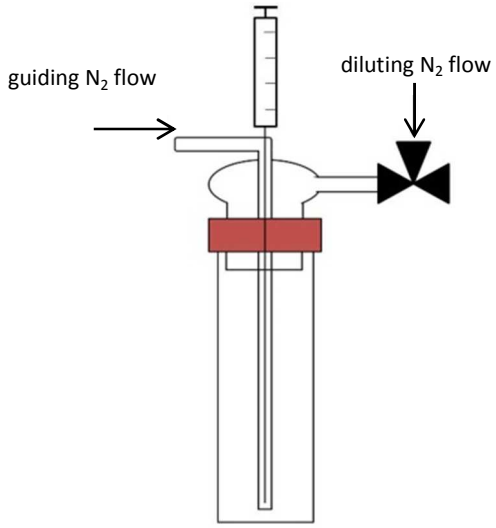

Figure S2: Adapted reactor for applying higher 1,2-DCE feeding rates with a perfusor pump

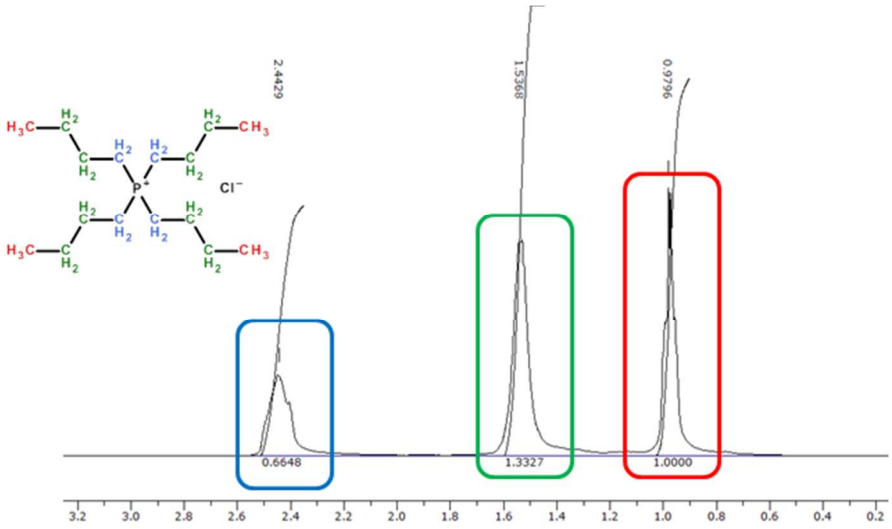

Figure S3: ^{1}H-NMR spectrum of $C_{4444}P^{+}Cl^{-}$ after reaction at 240 °C for 50 hours in $CDCl_3$. The integrated peak areas correspond to a $C_{4444}P^{+}Cl^{-}$ sample which has not suffered any measurable degradation.

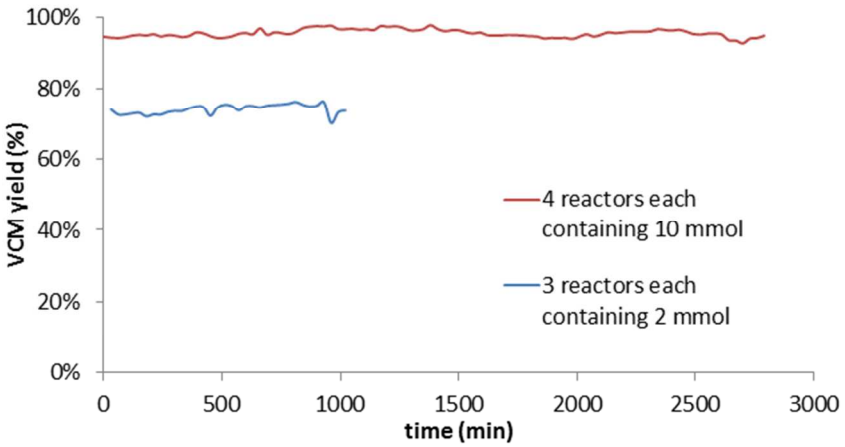

Figure S4: VCM yield (%) in function of reaction time (min) for reactions at 240 °C with $C_{4444}P^{+}Cl^{-}$. In one case 3 reactors were used in series each containing 2 mmol ionic liquid, to yield 75% VCM; in the other case 4 reactors were used in series each containing 10 mmol, to yield 93% VCM. Both reactions proceeded with a selectivity > 99.5%.