

Double Decarbonylation of Terephthaloyl Chloride: A Dual Versatile Route to *para*-Dichlorobenzene in Liquid and Gas Phases

Antoine Beuque^{1,*}, Marc-Olivier Simon², Emmanuel Marx², Jeremie Zaffran³, Pierre de Frémont³, Sergio Mastroianni², Stéphane Jeol²

¹Syensqo, Research and Innovation Center of Shanghai, Eco-Efficient Products and Processes Laboratory, 3966 Jindu Road, Xinzhuang Industrial Zone, Shanghai, China

²Syensqo, Research and Innovation Center of Lyon, 85 avenue des Frères Perret, 69190 Saint-Fons, France

³Centre National de la Recherche Scientifique, Eco-Efficient Products and Processes Laboratory, IRL 3464, 3966 Jindu Road, Xinzhuang Industrial Zone, Shanghai, China

Orcid Numbers:

Jeremie Zaffran: 0000-0003-3176-6140

Pierre de Frémont : 0000-0001-8470-3659

*Corresponding author: antoine.beuque@syensqo.com

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- Figure S4:** Calibration curves of TdCl and 4-CBCl analyzed by LC UV DAD and CIB, 4,4-DCIBP, and *p*-DCB analyzed by GC-FID.
- Figure S5:** Proposed mechanism for the homogeneous decarbonylation of TdCl with the Wilkinson's catalyst.
- Figure S6:** Figure S6: Products distribution and TON (*p*-DCB) obtained with 3.3 wt% Pd/C. The same experiment was repeated 4 times. Experimental conditions: 360 °C, 366 mg h⁻¹ of TdCl, 100 ml min⁻¹ N₂, 1 hour, WHSV (25 h⁻¹), 1 atm. The calculated sum of the product yield is considered as the conversion of TdCl.
- Figure S7:** Proposed block scheme of the production of *p*-DCB from terephthalic acid. Chlorination of terephthalic acid to terephthaloyl chloride followed by decarbonylation to *p*-DCB.
- Table S1:** Estimation of the TdCl flow rate after bubbling in N₂ during 1 hour
- Table S2:** Recap table of the catalysts used in the literature for aroyl chloride decarbonylation.
- Table S3:** Pd and Cl amount calculated by XRF analysis using semi-quantitative techniques on the 3.3 wt% Pd/C catalyst.

1. General

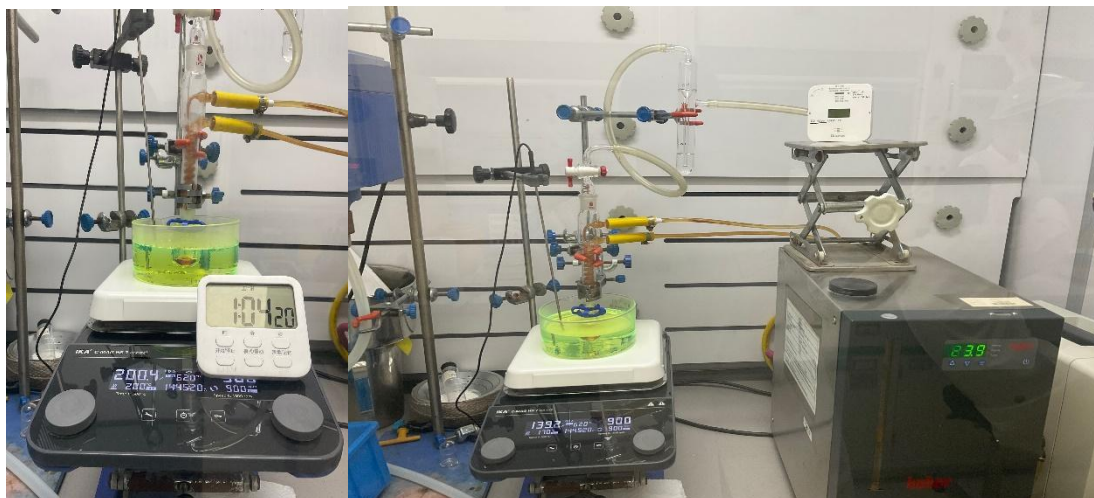


Figure S1: Experimental setup for the liquid phase decarbonylation of TdCl.

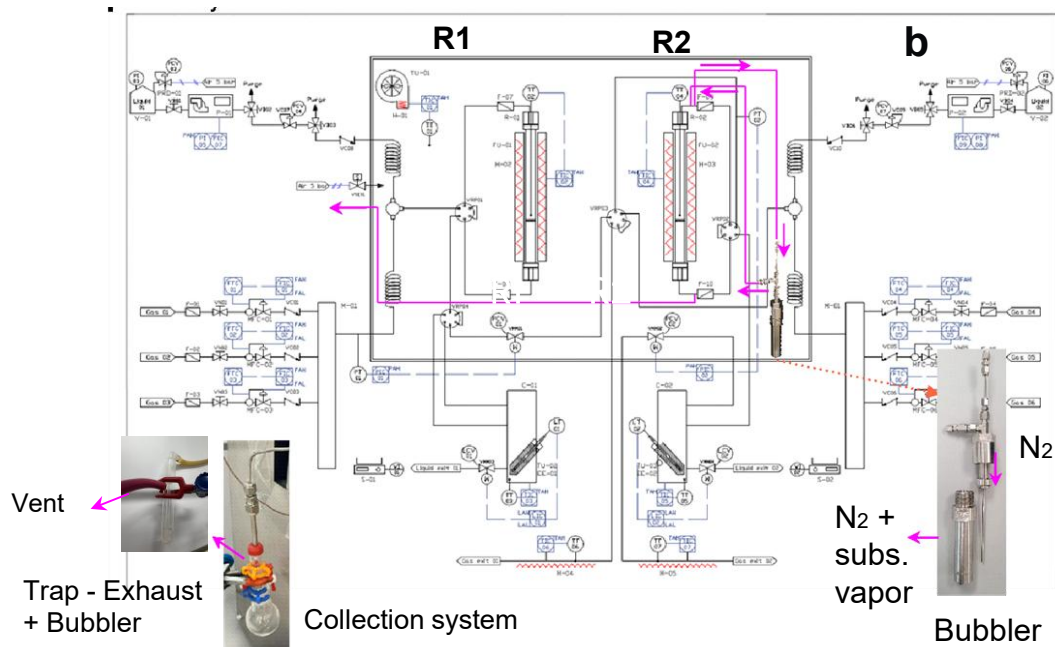


Figure S2: (a) Modified EFFI microactivity FR 200 reactor from Micromeritics and (b) PID of the experimental for the gas phase decarbonylation of TdCl.

The heterogeneous catalytic decarbonylation of TdCl is carried out in the gas phase. Due to the high melting point (83 °C) and boiling point (259 °C) of TdCl, it leads to technical challenges. To remediate this issue, a EFFI microactivity FR 200 reactor from Micromeritics was slightly modified and then used in the gas phase catalytic reaction.

The system consists of a hotbox that can be closed/opened and heated (box-T). Inside the box, two parallel reactors are present that can be separately heated (R1-T and R2-T). In the control software of the Micro-Effi make sure that the operation mode is "PARALLEL - OPTION 1. At the inlet of reactor 2

(R2), a bubbler was installed inside the hotbox. The substrate TdCl was loaded inside the bubbler to bubble nitrogen through the TdCl. Attach the end of the gas line to the collection system composed by a schlenk and a secondary trap both refrigerated properly outside the box. The secondary trap is connected to a liquid bubbler (e.g. filled with mineral oil). The exhaust gas is finally directed to the vent (Figure S2).

The stainless-steel reactor column (R2) with an inner diameter of 1 cm is loaded with the required amount of catalyst (100 - 300 mg). Similarly, the stainless-steel bubbler is loaded with 4 g of TdCl inside the glovebox and transferred to the Effi microactivity system. A nitrogen flow of 100 ml min⁻¹ is set to keep the catalyst and substrate under the inter atmosphere.

Before the reaction, a gas leak-check is carried out. A Swagelok cap/plug is attached at the outlet of the reactor and the system is pressurised with 5 bars of N₂. After 5 minutes of pressurization, the pressure in the system is noted to confirm the pressure stability or pressure drop. Once the pressure is stable, reconnect the outlet of the reactor to the collection system, close the hotbox and stop the N₂ flow.

The hotbox is heated to 200 °C, (the thermocouple connected outside the bubbler indicates 160 °C), the reactor 2 to the reaction temperature (360 °C) and the external line to 250 °C. When the thermal equilibrium is reached, open the N₂-flow to 100 ml/min at 1 atm. A pressure gauge was installed at the reactor inlet to monitor the pressure system online. This is the beginning of the reaction noted t₀. Confirm the gas flow by inspecting the liquid bubbler at the end of the collection system.

After 1 hour of reaction, the heating of the hotbox, reactor and external lines is stopped, set to room temperature and the hotbox opens to favor a rapid quenching of the reaction (5 min to 30 °C inside the boiler, below the melting point of TdCl). Continue to purge the system from residual CO with the N₂-flow (N₂-flow = 100 ml/min). After 10 min of N₂ purge, stop the N₂ flow (N₂-flow = 0 ml/min). The collection system can be disassembled for analysis of reaction products collected in the Schlenk. The spent catalyst is also recovered for analysis.

Similarly to the liquid phase reaction, the crude sample is dissolved in 25 mL in DCM for GC analysis (CS25). Then, the solution is further diluted by a factor 50 in DCM to prepare for LC injection (CD50).

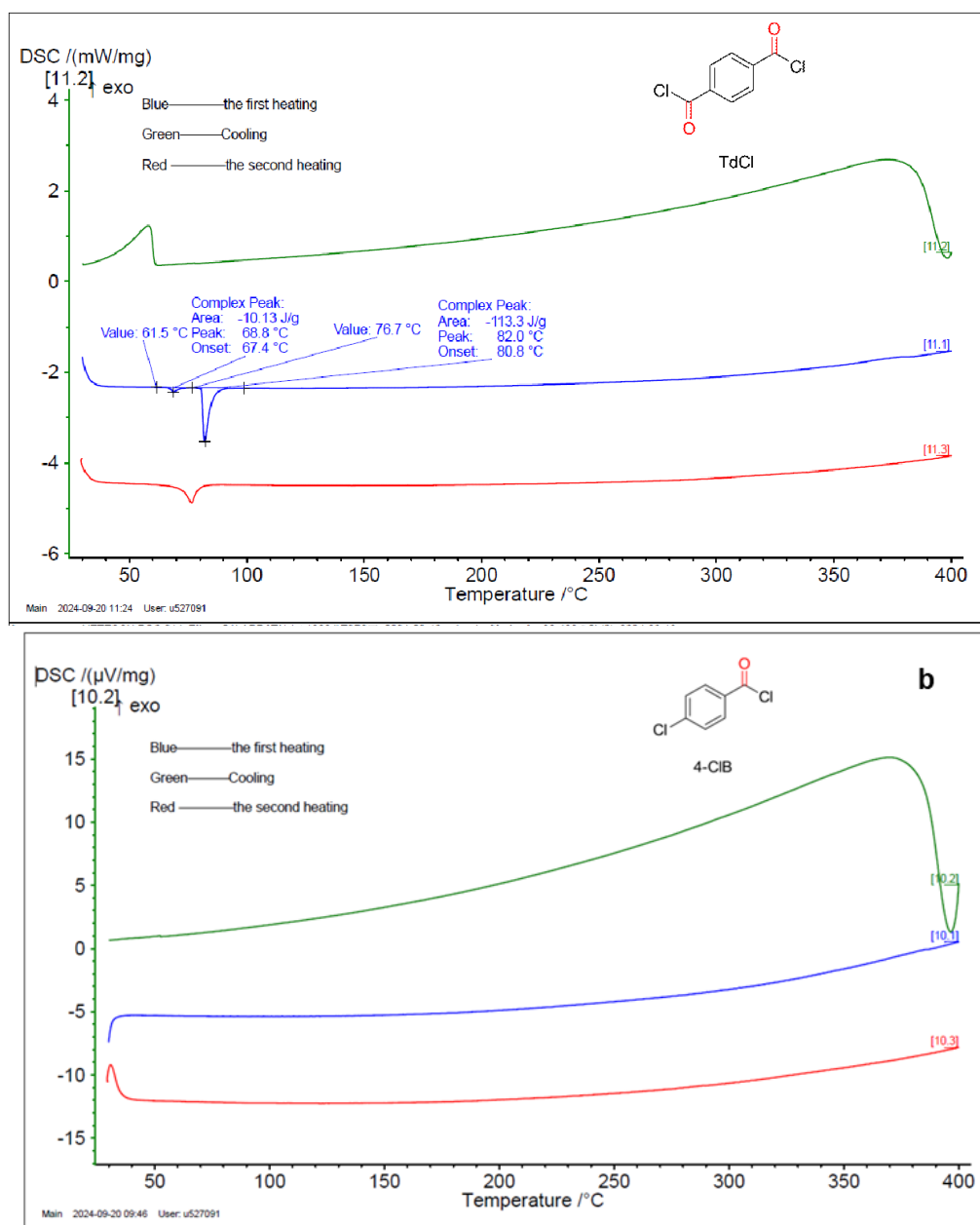


Figure S3: Differential scanning calorimetry of TdCl (a) and 4-CIB (b) from room temperature to 400 °C.

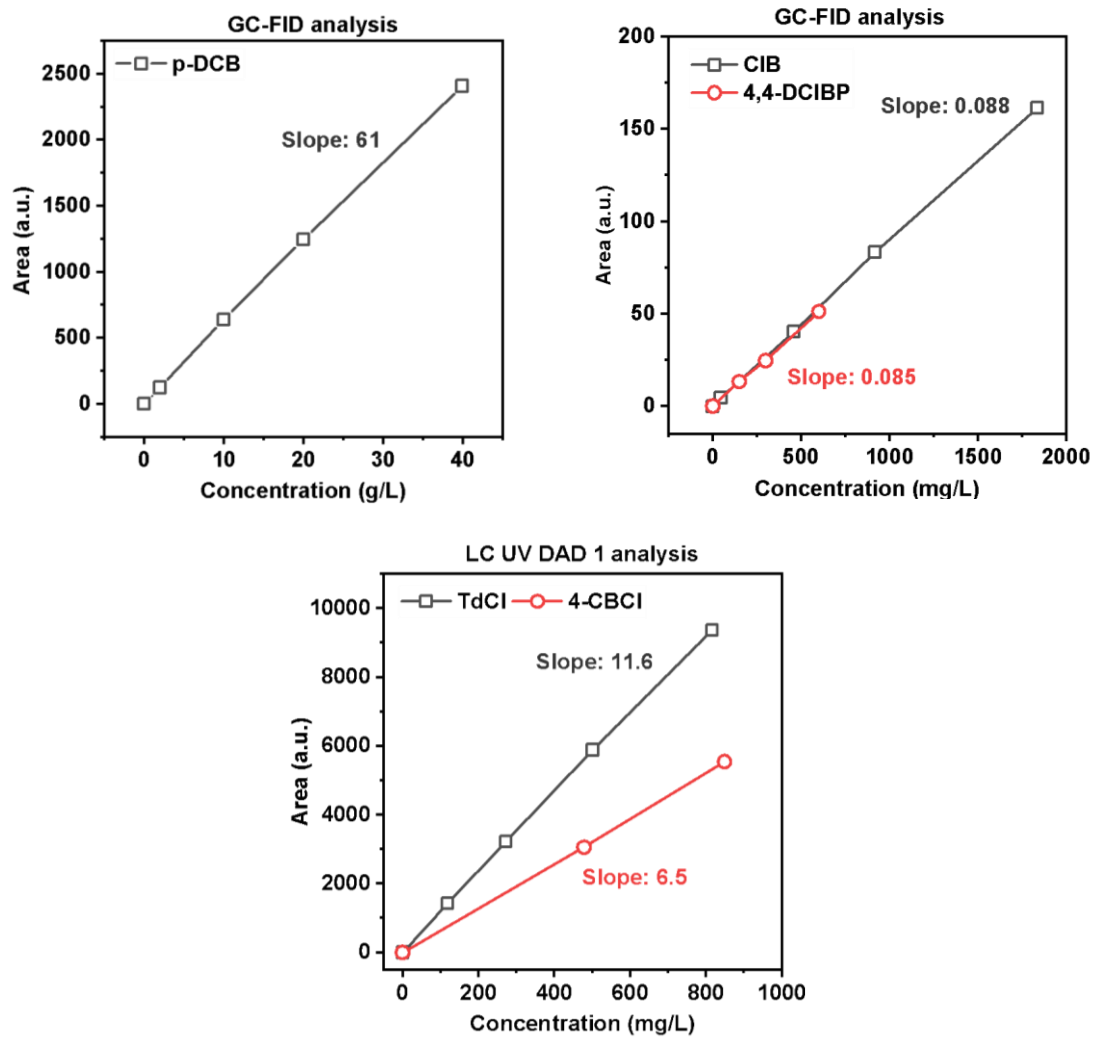
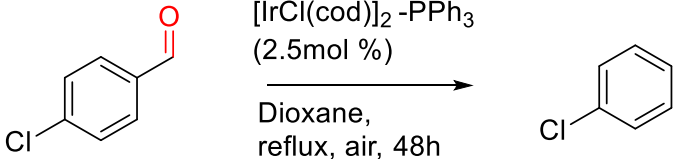
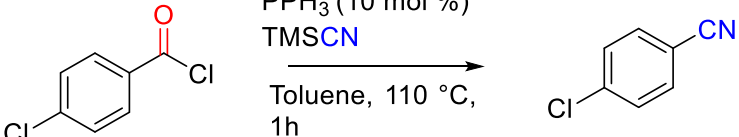
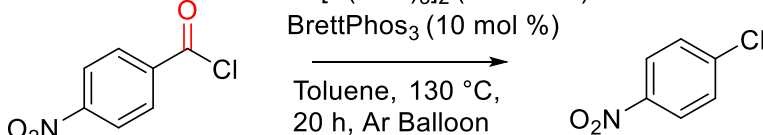
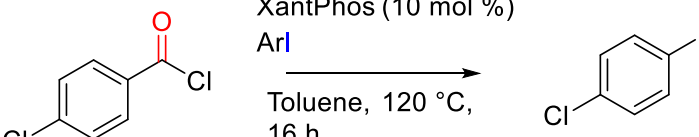


Figure S4: Calibration curves of TdCl and 4-CBCl analyzed by LC UV DAD and CIB, 4,4-DCIBP, and p-DCB analyzed by GC-FID.

Table S1: Estimation of the TdCl flow rate after bubbling in N₂ during 1 hour

Hotbox temperature (°C)	Bubbler temperature (°C)	Reactor temperature (°C)	N ₂ flow rate (ml h ⁻¹)	Pressure drop (bar)	TdCl flow rate (mg h ⁻¹)
200	160	360	100	0.7	420
					359
					320

Table S2: Recap table of the catalysts used in the literature for aroyl chloride decarbonylation.

Catalytic system		Reaction		Ref
Name	Ligand	Scheme	Yield (%)	
[IrCl(cod)] ₂	PPh ₃	 <p>[IrCl(cod)]₂-PPh₃ (2.5 mol %) Dioxane, reflux, air, 48h</p>	79	25
Ni(cod) ₂	BrettPhos	 <p>[Ni(cod)]₂ (20 mol %) PPh₃ (10 mol %) TMS-CN Toluene, 110 °C, 1h</p>	96	26
Pd[P(o-tol) ₃] ₂	BrettPhos	 <p>Pd[P(o-tol)₃]₂ (20 mol %) BrettPhos₃ (10 mol %) Toluene, 130 °C, 20 h, Ar Balloon</p>	82	27
Pd ₂ (dba) ₃	Xantphos	 <p>[Pd₂(dba)₃] (5 mol %) XantPhos (10 mol %) ArI Toluene, 120 °C, 16 h</p>	85	28-29

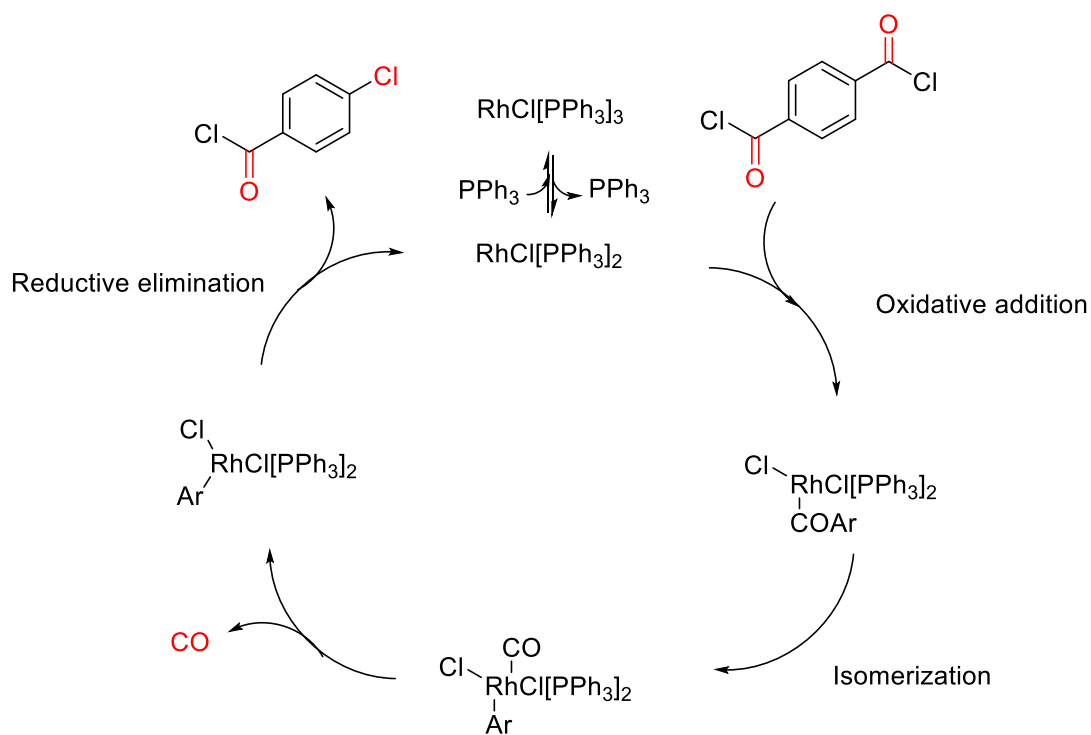
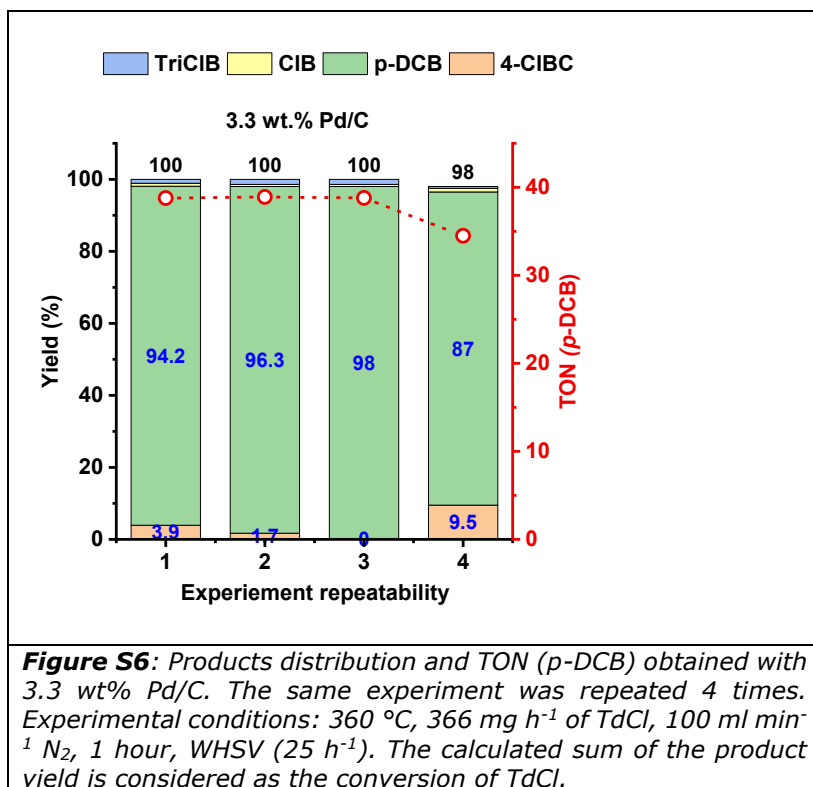


Figure S5: Proposed mechanism for the homogeneous decarbonylation of TdCl with the Wilkinson's catalyst.²²

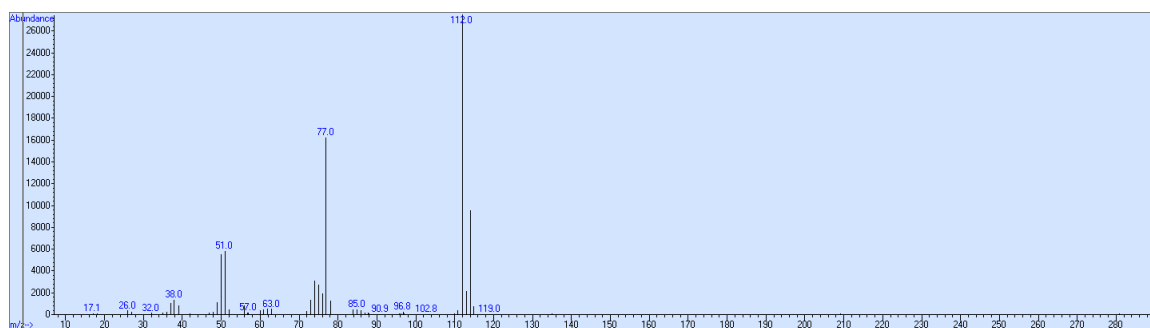
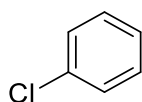
Table S3: Pd and Cl amount calculated by XRF analysis using semi-quantitative techniques on the 3.3 wt% Pd/C catalyst.

Catalyst state	Pd (wt%)	Cl (wt%)	Pd (mol%)	Cl(mol%)	Molar ratio Cl/Pd
Fresh	3.477	0.19	0.03267 24	0.00536	0.164042329
Spent	3.983	11.296	0.03742 72	0.318646	8.513759784
After DCM extraction	2.732	5.431	0.02567 19	0.153202	5.967688184



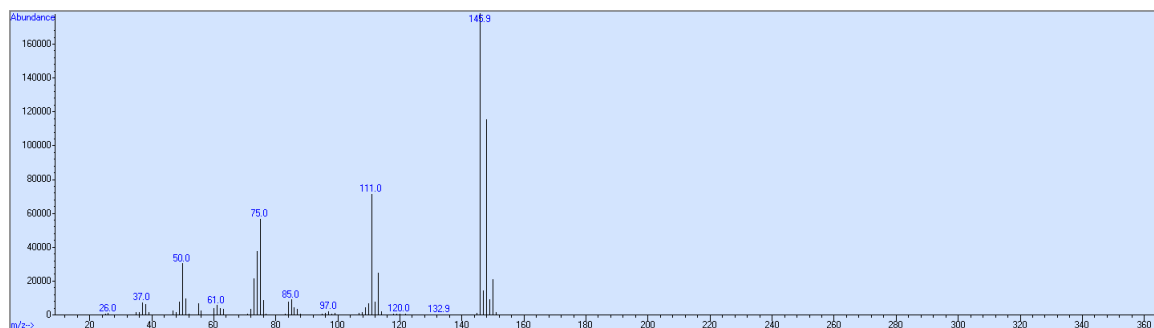
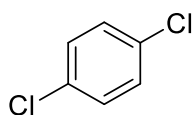
2. Product identification

Chlorobenzene (CIB), (MW = 112 g mol⁻¹)



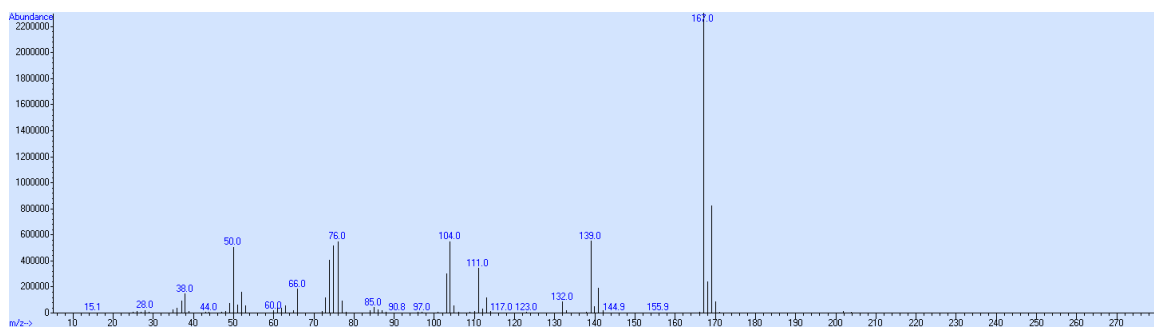
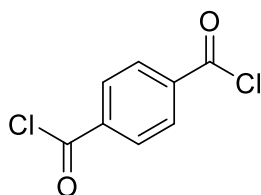
GC/MS (EI, 70 eV): m/z (rel. int., %): 38 (4), 50 (23), 51 (25), 74 (11), 75 (9), 76 (6), 77 (65), 112 (100), 113 (8), 114 (38)

Para-dichlorobenzene (p-DCB), (MW = 146 g mol⁻¹)



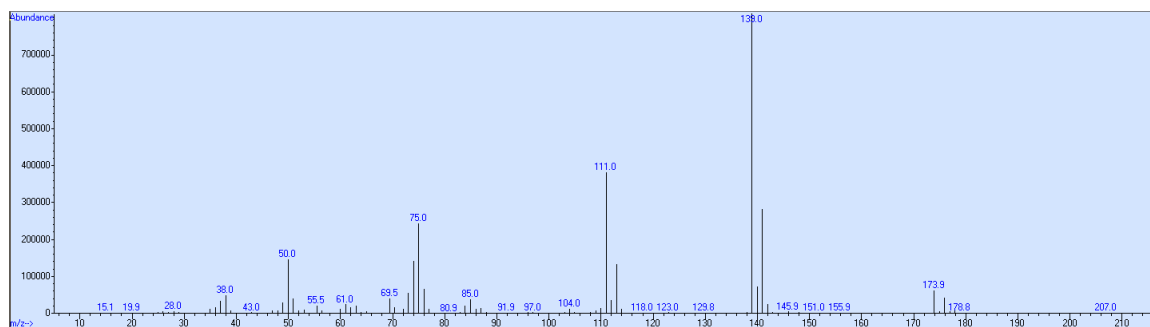
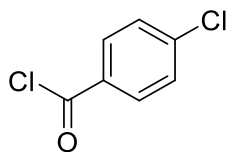
GC/MS (EI, 70 eV): m/z (rel. int., %): 50 (14), 73 (9), 74 (16), 75 (27), 111 (41), 113 (13), 146 (100), 147 (8), 148 (67), 150 (11)

Terephthaloyl chloride (TdCl), (MW = 220 g mol⁻¹)



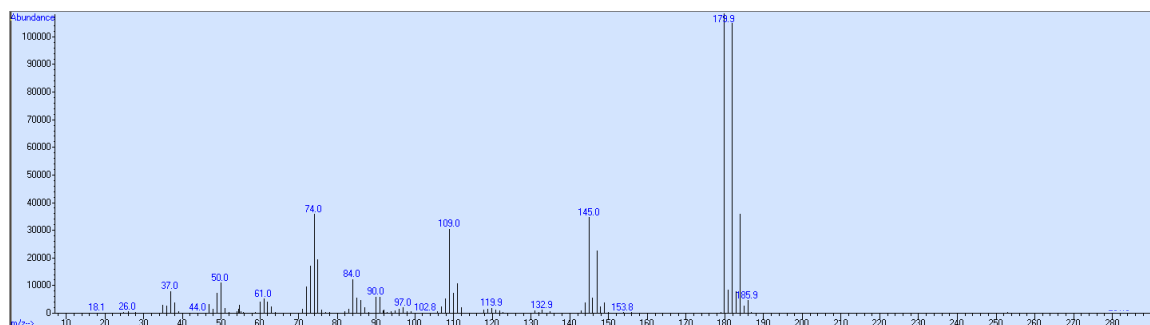
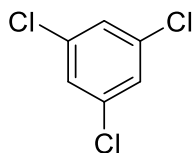
GC/MS (EI, 70 eV): m/z (rel. int., %): 50 (20), 74 (16), 75 (20), 76 (20), 103 (12), 104 (21), 111 (15), 139 (22), 167 (100), 169 (33)

4-Chlorobenzoyl chloride (4-CIBC), (MW = 174 g mol⁻¹)



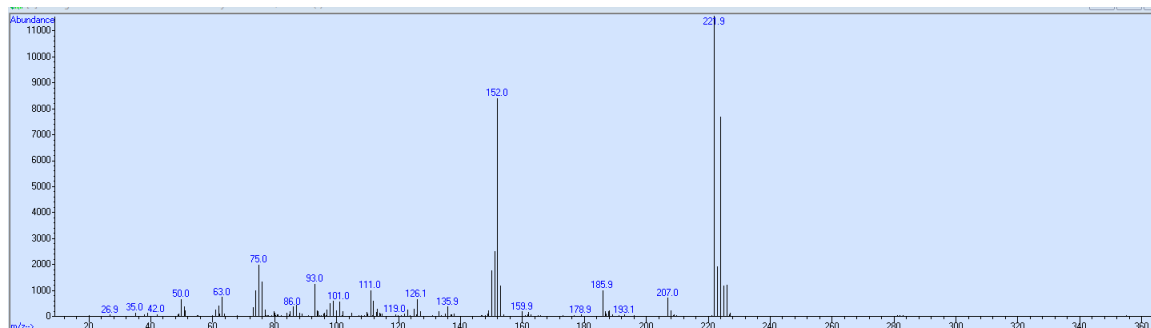
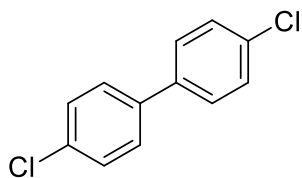
GC/MS (EI, 70 eV): m/z (rel. int., %): 50 (12), 74 (12), 75 (25), 111 (49), 113 (15), 139 (100), 140 (9), 141 (32), 174 (11), 176 (7)

Trichlorobenzene (TriCl), (MW = 180 g mol⁻¹)



GC/MS (EI, 70 eV): m/z (rel. int., %): 73 (11), 74 (25), 75 (14), 109 (25), 111 (8), 145 (33), 147 (22), 180 (100), 182 (95), 184 (31)

4,4-Dichlorobiphenyl (4,4 DCIBP), (MW = 222 g mol⁻¹)



GC/MS (EI, 70 eV): m/z (rel. int., %): 74 (10), 75 (22), 76 (11), 150 (14), 151 (21), 152 (72), 222 (100), 223 (15), 224 (62), 226 (10)

3. Modelling supplementary Information

1- Structure coordinates

Below are reported, in .vasp format, the structure coordinates related to Cl adsorbate deposited onto Pd (111), Al₂O₃ (110) and C (001).

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4. Methodology for integrated Techno-Economic Assessment (TEA) and Life Cycle Assessment (LCA)

The objective is to estimate its Full Manufacturing Cost (FMC) - which comprises Variable Costs, Depreciation of the Capex and Fixed Costs - and its environmental footprint. The methodology is structured as follows:

4.1. Construction of evolutive Material Balance and Process Block Diagram

This first step involves building a detailed material balance, which is parameterized and thus evolutive. This means the model can be easily updated as new data becomes available or as process parameters change. The material balance is developed in close collaboration with the project's chemists, using their experimental data and process insights. In parallel, a process block diagram is constructed to visually represent the main process steps and material flows, including recycling solvents or unreacted raw materials when needed. When specific information is missing, standard industrial assumptions or

data from the literature on similar processes are used to ensure continuity and robustness in the analysis..

4.2. Calculation of Unit Consumption, Variable Costs and Ecoprofile

Based on the material balance, the consumption or generation of raw materials, utilities, wastes and other inputs or outputs per unit of product are calculated. The database used is Ecoinvent V3.11 - allocation cut-off by classification.

4.2.a Variable Costs

Using the calculated unit consumptions together with current market prices or project-specific cost data, the variable costs are estimated. This approach enables a transparent and detailed breakdown of the cost structure, clearly identifying the main cost drivers.

4.2.b Ecoprofile

In parallel, the same unit consumption data is used together with Life Cycle Assessment (LCA) results for each input and output to calculate the overall environmental profile (ecoprofile) as the sum of the individual contributions. This analysis provides a detailed breakdown of environmental impacts, highlighting the main hotspots across the various impact categories assessed by the chosen LCA method, such as Global Warming Potential (GWP) or Human Toxicity.

This dual approach ensures that both economic and environmental performance are evaluated consistently and transparently, supporting informed decision-making and targeted process improvements.

4.3. Estimation of Depreciation

The process block diagram serves as the basis for estimating the capital expenditure (Capex) required to build the production facility. An internal Syensqo tool, specifically adapted for early-stage research projects, is used to generate a preliminary Capex estimate. This Capex is then depreciated over a specific period of time, giving the Depreciation. This approach ensures that the estimate is aligned with the maturity of the project and the available information.

4.4. Estimation of Fixed Costs

Fixed costs include costs such as labor, maintenance, overheads, and other expenses that do not vary directly with production volume. They are estimated using internal Syensqo benchmarks and/or industry-recognized rules of thumb.

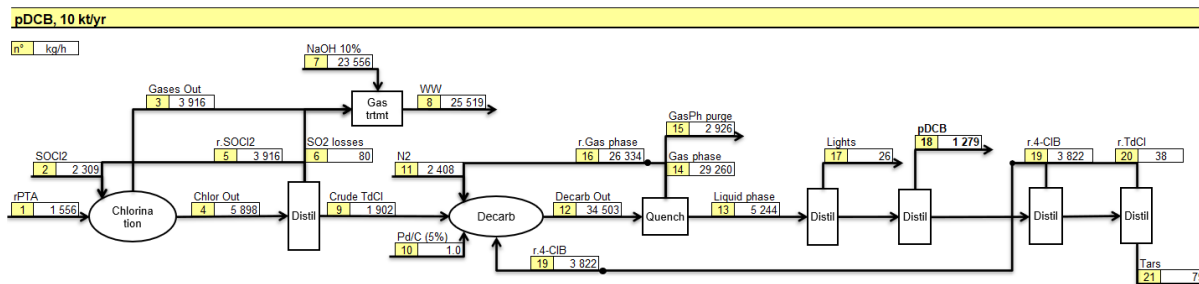


Figure S7: Proposed block scheme of the production of p-DCB from terephthalic acid. Chlorination of terephthalic acid to terephthaloyl chloride followed by decarbonylation to p-DCB.