Electronic supplementary materials *Mendeleev Commun.*, 2025, **35**, 353–355

Dechlorination of 1,4-dichlorobenzene on unsupported nickel phosphides synthesized *in situ*: effect of Ni/P ratio on the catalyst activity

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The nanoheterogeneous catalysts were prepared using nickel 2-ethylhexanoate (≥78%, cat. no. 338184, Sigma-Aldrich) as the precursor. The substrate used was 1,4-dichlorobenzene (≥99%, cat. no. 106467, Sigma-Aldrich). The solvent used was *n*-hexadecane (≥98%, Component-Reactiv PJSC), and a 10% solution of 1,4-dichlorobenzene was prepared.

The catalysts were synthesised *in situ* in the reaction medium in a batch reactor, under constant stirring at 340 °C and a H_2 pressure of 6 MPa (≥98%, Air Liquide) for a period of 7 hours. The phosphidation agent was either red phosphorus or triphenylphosphine (≥99%, Component-Reactiv PJSC), and the molar ratio of P/Ni was varied from 0 to 20. The molar ratio of catalyst to substrate is 60. The conditions of the catalytic experiments are the same as those used for the synthesis of the catalyst, as the catalyst was synthesised *in situ*. 1,4-dichlorobenzene was used as a substrate to model the liquid pyrolysis products of polymer waste mixtures.

The products were analysed by gas chromatography on a chromatograph 'Crystallux-4000M' (LLC 'NPF 'Meta-Chrom') with a capillary column Optima 1 (30 m × 0.32mm × 0.50μm).

The phase composition of the catalysts was determined by means of powder X-ray diffraction. X-ray diffractograms were obtained for a range of 5–100° 2θ using a Rigaku Rotaflex RU-200 diffractometer (CuKα radiation) equipped with a Rigaku D/Max-RC goniometer (a rotation speed of 1°/min; a step 0.04°). Qualitative phase analysis of the samples was conducted using the PDF-2 ICDD database of powder diffraction patterns.