Supplementary Information for

Monodisperse Palladium-Cobalt Alloy Nanoparticles Assembled on Poly (N-vinyl-pyrrolidone) (PVP) as Highly Effective Catalyst for the Dimethylammine Borane (DMAB) dehydrocoupling

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Materials

Aldrich supplied superhydride, dimethylamine-borane, $CoCl_2$, K_2PdCl_4 and poly(N-vinyl-2-pyrrolidone). C_2H_5OH and water used during this study were provided from Merck and Milli Q-pure machine, respectively. Before washing all glass pieces and other lab materials with large amount of distilled water, they were cleaned with acetone, then dried.

Analytical investigations of Pd-Co@PVP NPs

TEM samples were made ready by dropping of 0.5 mg/mL ethanol solution of the prepared catalysts with an activated carbon support on a carbon covered 400-mesh copper grid, and then the solvent was vaporized. Elimination of excess solution was performed with an adsorbent paper and the sample was dried under vacuum at room temperature before analysis. TEM analysis was carried out by a JEOL 200 kV. More than 300 particles were calculated to get the integrated information about the overall distribution of Pt-based catalyst sample.

During X-ray Photoelectron Spectroscopy (XPS) analysis, Specs spectrometer was employed and as an X-ray source Kα lines of Mg (1253.6 eV, 10 mA) was used. Sample preparation was done by depositing the catalyst on Cu double-sided tape (3M Inc.). C 1s line at 284.6 eV was selected as a reference point and all XPS peaks were fitted using a Gaussian function and the C 1s line at 284.6 eV was used as the reference line.

XRD analysis were performed with a Panalytical Empyrean diffractometer with Ultima+theta–theta high resolution goniometer, having an X-ray generator (Cu K∞ radiation, k = 1.54056 Å) and operating condition of 40 kV and 40 mA.

UV–Vis analyses were taken by Perkin Elmer Lambda 750. 200–900 nm was selected to gather the data and 1 cm-long a quartz cell was employed.

^{11}B NMR spectra were recorded on a Bruker Avance DPX 400 MHz spectrometer (128.2 MHz for ^{11}B NMR).

Investigation of performances of Pd-Co@PVP NPs during DMAB dehydrogenation

By means of the rate of hydrogen emission, the performance of Pd-Co@PVP NPs during dehydrogenation of DMAB was examined. During the study, a coated vessel (50 mL) was put on stiring machine and kept the reaction temperature 25.0 ± 0.1◦C by flowing H_2O in special parts of reaction vessel from a bath where temperature was fixed. After that,water was poured into a millimetric glass pipe (50 cm in height and 4.0 cm in size) and attached to the dehydrogenation chamber to find the amount of H_2 generated. In a sample work, DMAB was transported into the reaction chamber with 25.0 ± 0.1◦C of fixed temperature. After transferring same amount of Pd-Co@PVP NPs, dehydrogenation of DMAB was began by covering the reaction chamber and the amount of H_2 fabricated was found writing H_2O change in the column at 1000 round per minute. Also, by ^{11}B NMR, the change of DMAB ($\delta = -12.6$ ppm) to $(Me_2NBH_2)_2$ ($\delta = 5.0$ ppm) was discovered, besides measuring the amount of hydrogen gas.

Reusability examination of Pd-Co nanomaterials stabilized by PVP

Some amount of PVP-stabilized Pd-Co nanomaterials (0.3 mM) was placed to get 20 mL of solution. This mixture and 100 mM DMAB was employed to measure the usage performance of PVP-stabilized Pd-Co nanocatalyst during the reaction of DMAB at 25.0 ± 0.1◦C. Several experiments was carried out for this purpose. After the completion of DMAB change to metaborate, equal amount of DMAB was placed again to the reaction chamber suddenly. The data were written as % starting performance of Pd-Co nanomaterials stabilized by PVP versus the number of catalytic cycles during DMAB dehydrogenation.

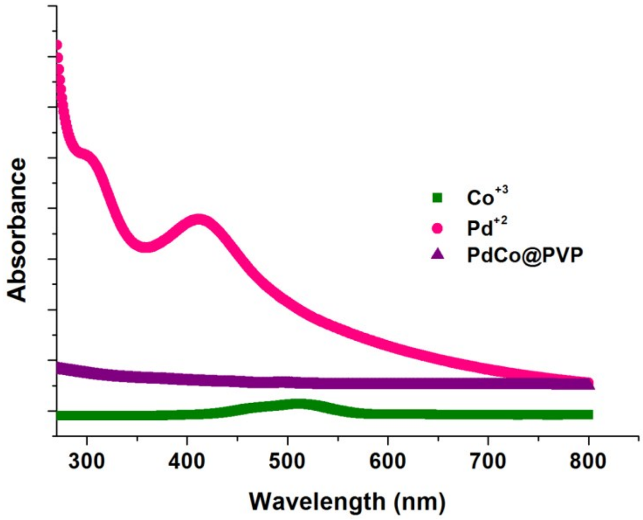

Fig. S1. UV-Vis absorption spectra of the aqueous solutions of Pd^{+2}, Co^{+3}, and Pd-Co@PVP NPs

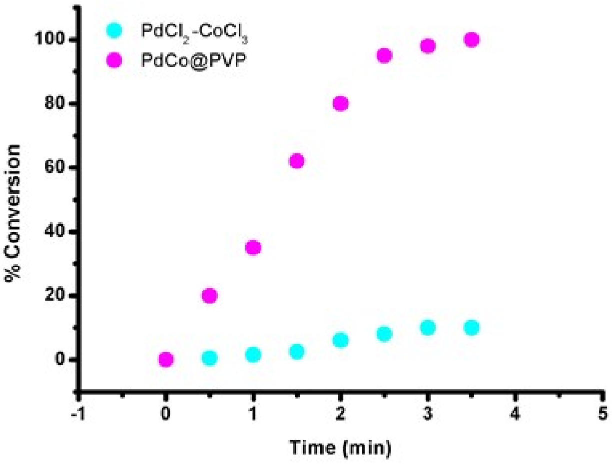

Fig. S2. Plots % conversion versus time graph for the catalytic dehydrocoupling of DMAB in THF at room temperature starting with 7.5 % mol of Pd-Co@PVP NPs and $PdCl_2$-$CoCl_3$ mixture

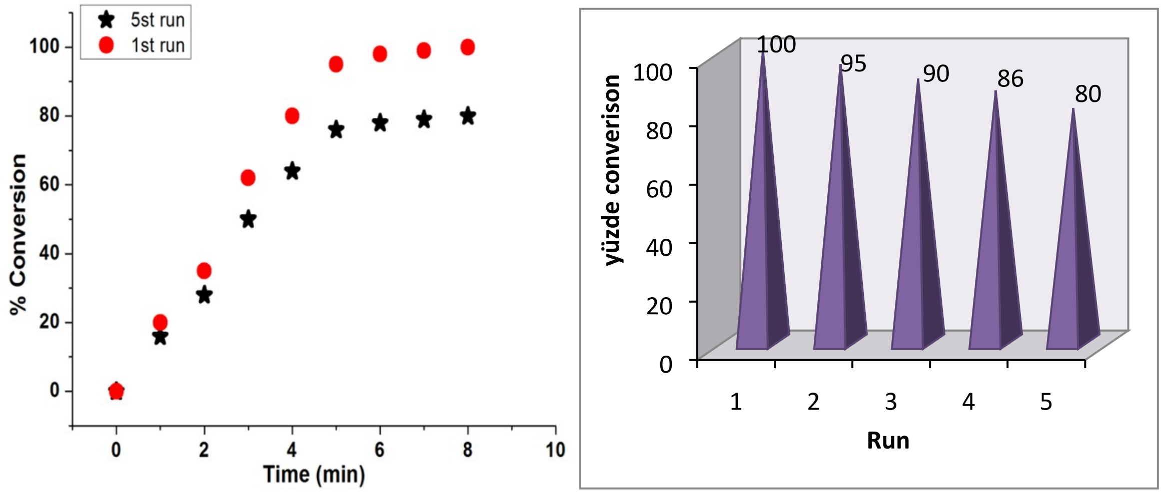

Fig. S3. Plots % conversion versus time graph for Pd-Co@PVP NPs (7.5 % mol) catalysed dehydrocoupling of DMAB in THF at room temperature for 1st and 5th catalytic runs.

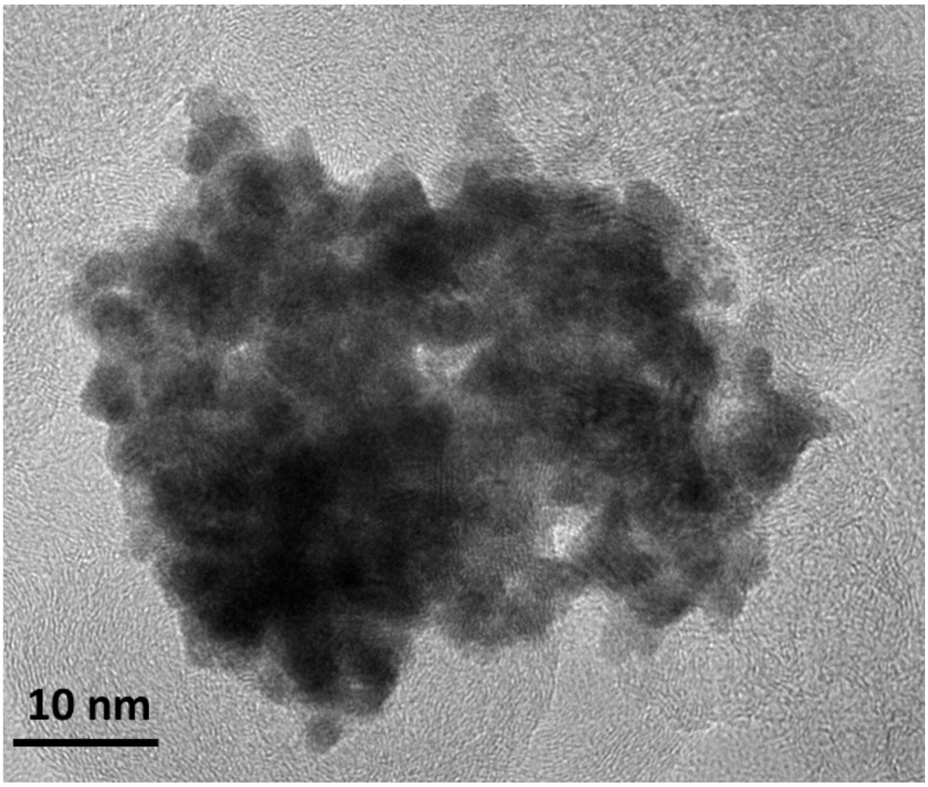

Fig. S4. TEM image of Pd-Co@PVP NPs after 5th catalytic runs.