Supporting Information

Tuning the metal valence state of Pd nanoparticles via codoping of B-N for chlorophenol hydrodechlorination

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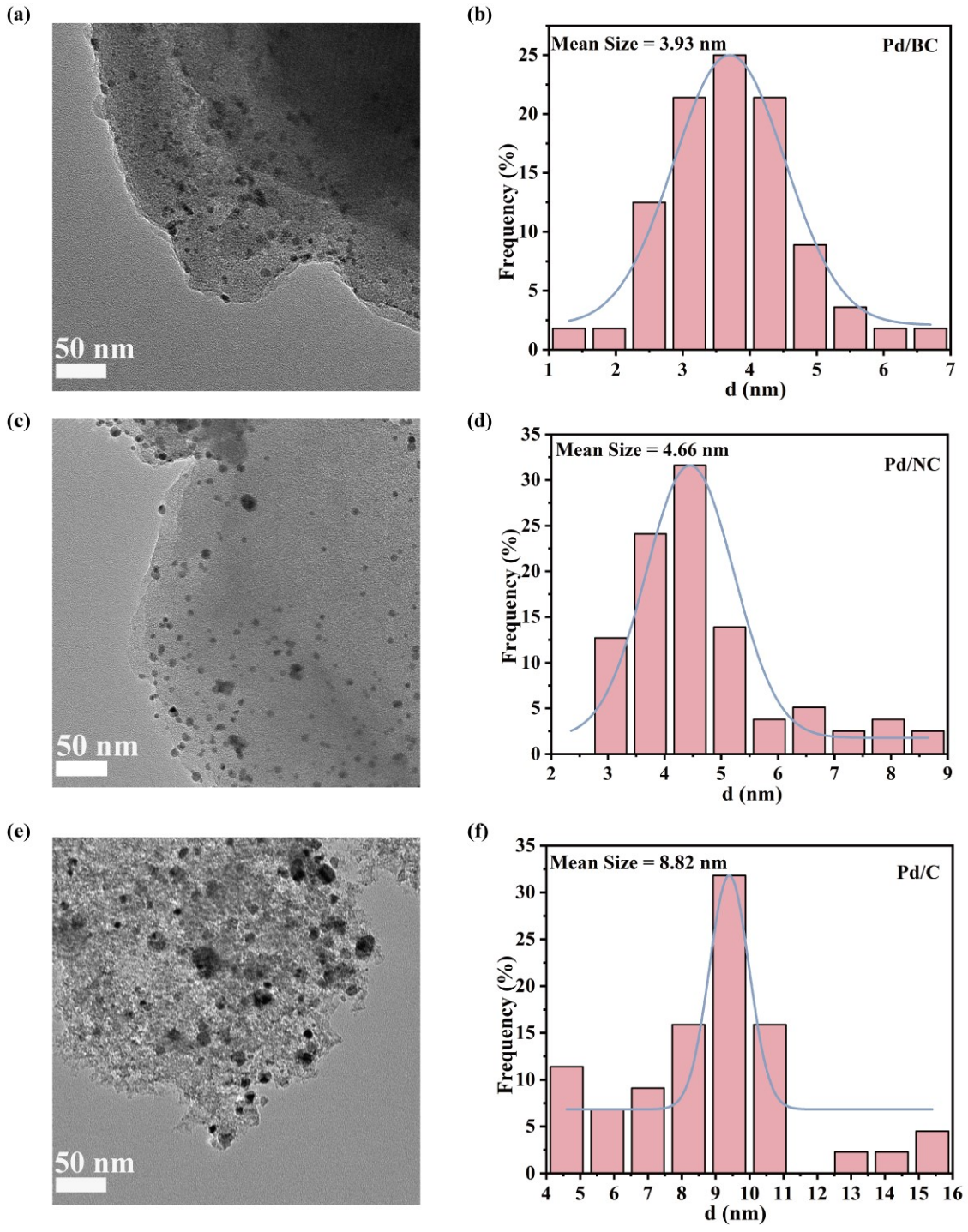


Figure S1 TEM images of Pd/BC (a), Pd/NC (c), and Pd/C (e) and the corresponding particle size distribution of Pd/BC (b), Pd/NC (d) and Pd/C (f), respectively.

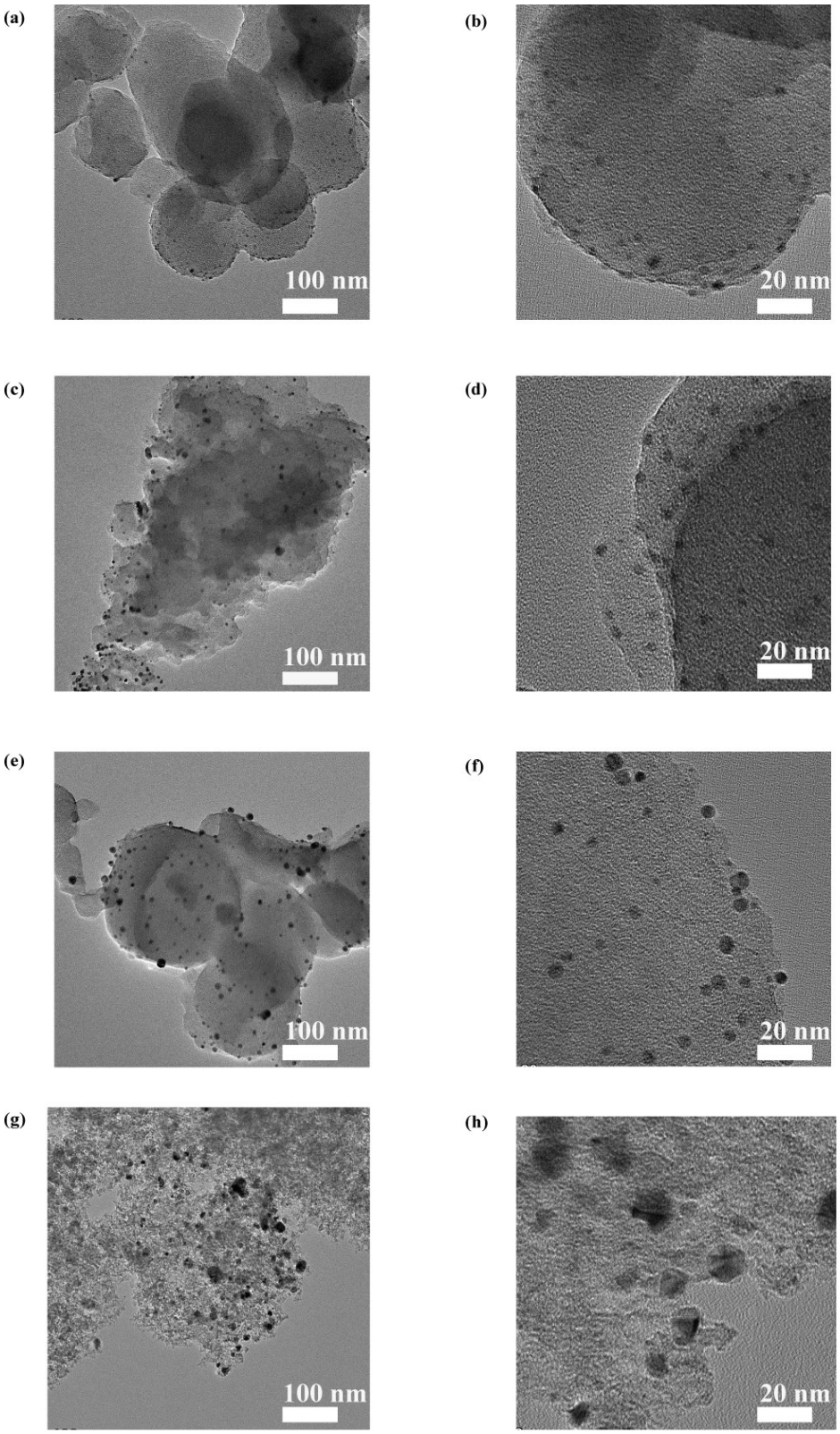
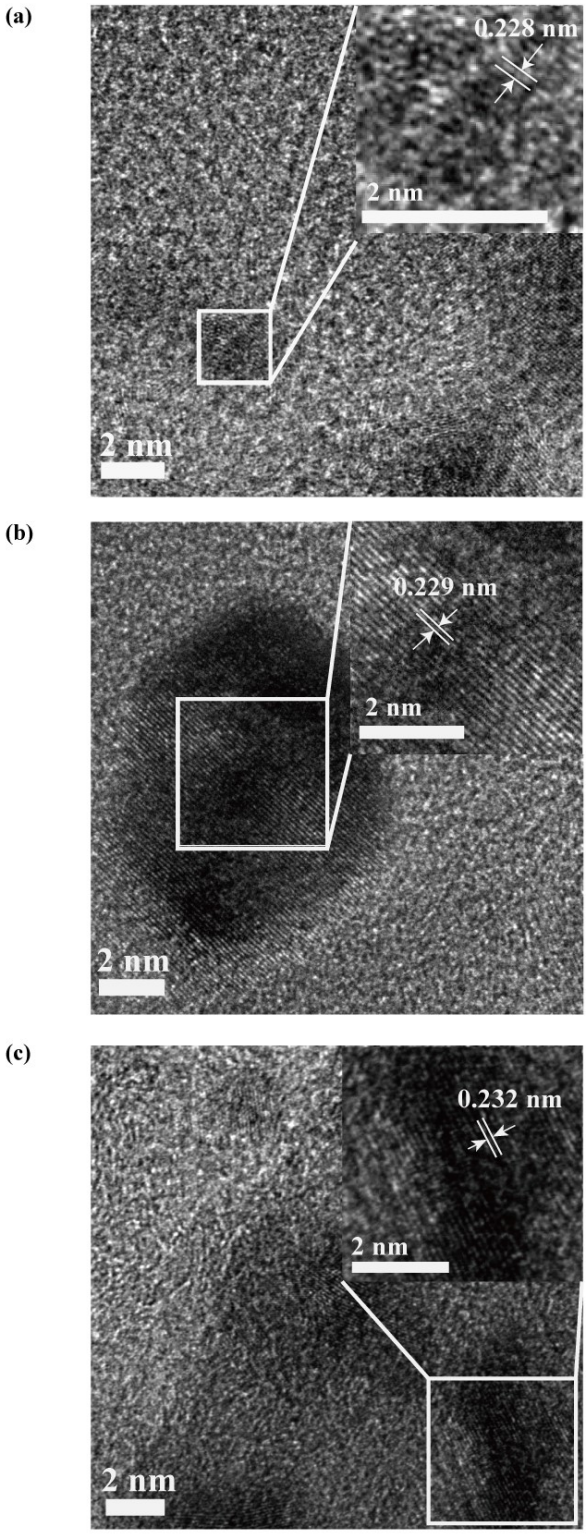


Figure S2 TEM images of Pd/BNC (a, b), Pd/BC (c, d), Pd/NC (e, f), and Pd/C (g, h) with scale around 100nm and 20nm.



b

Figure S3 HRTEM image of Pd/BC (a), Pd/NC (b), and Pd/C (c), respectively.

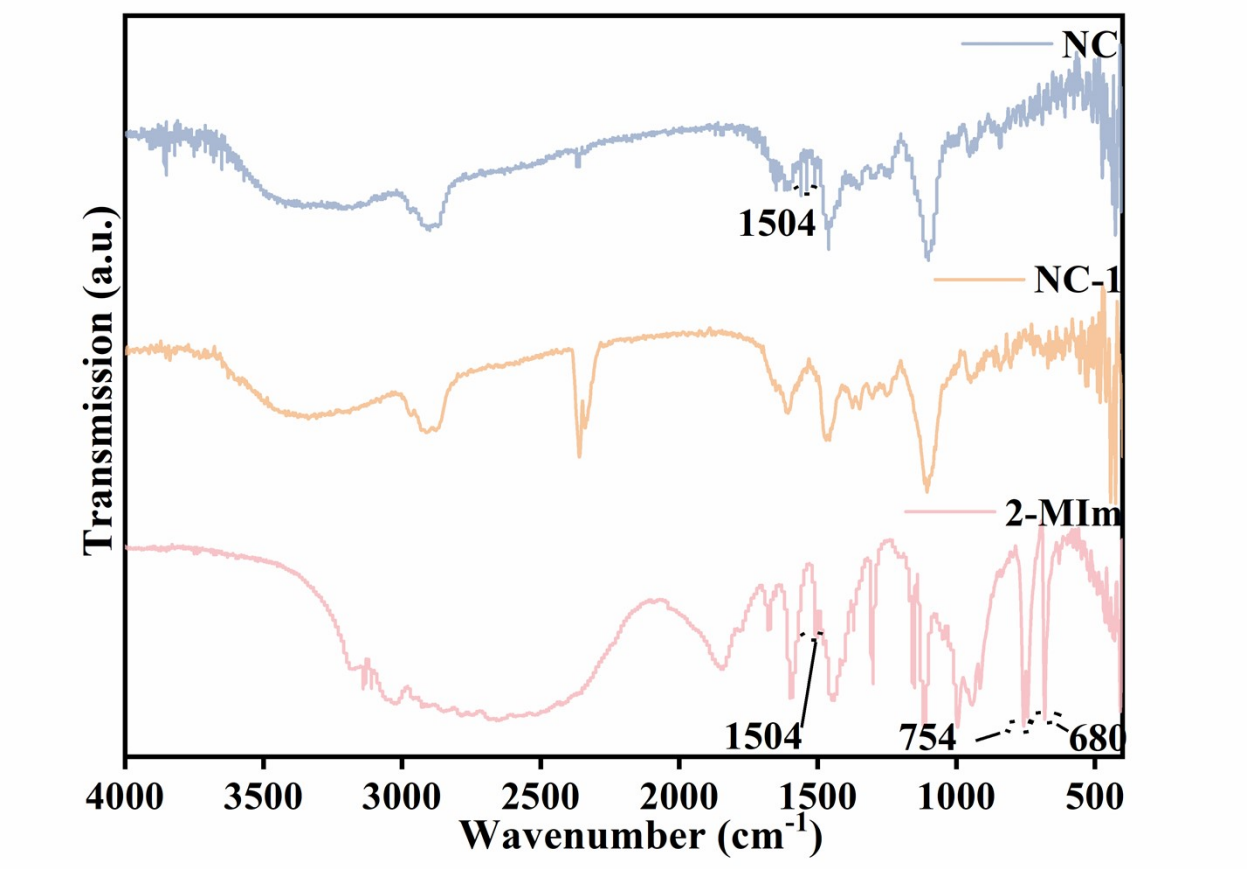


Figure S4 FT-IR spectra of as-NC and as-NC-1 compared with the FT-IR spectra of 2-MIm.

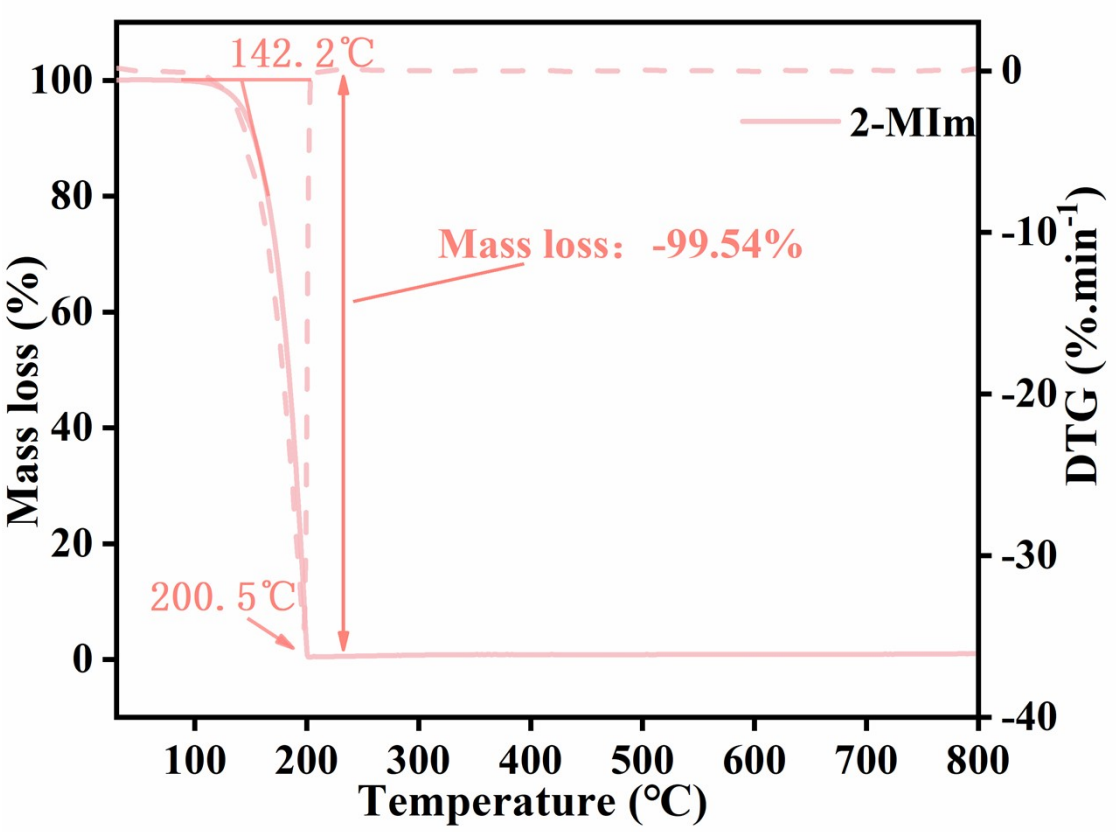


Figure S5 TGA curve of 2-methylimidazole. The solid line and dashed line represent the curve of mass loss and DTG with temperature, respectively.

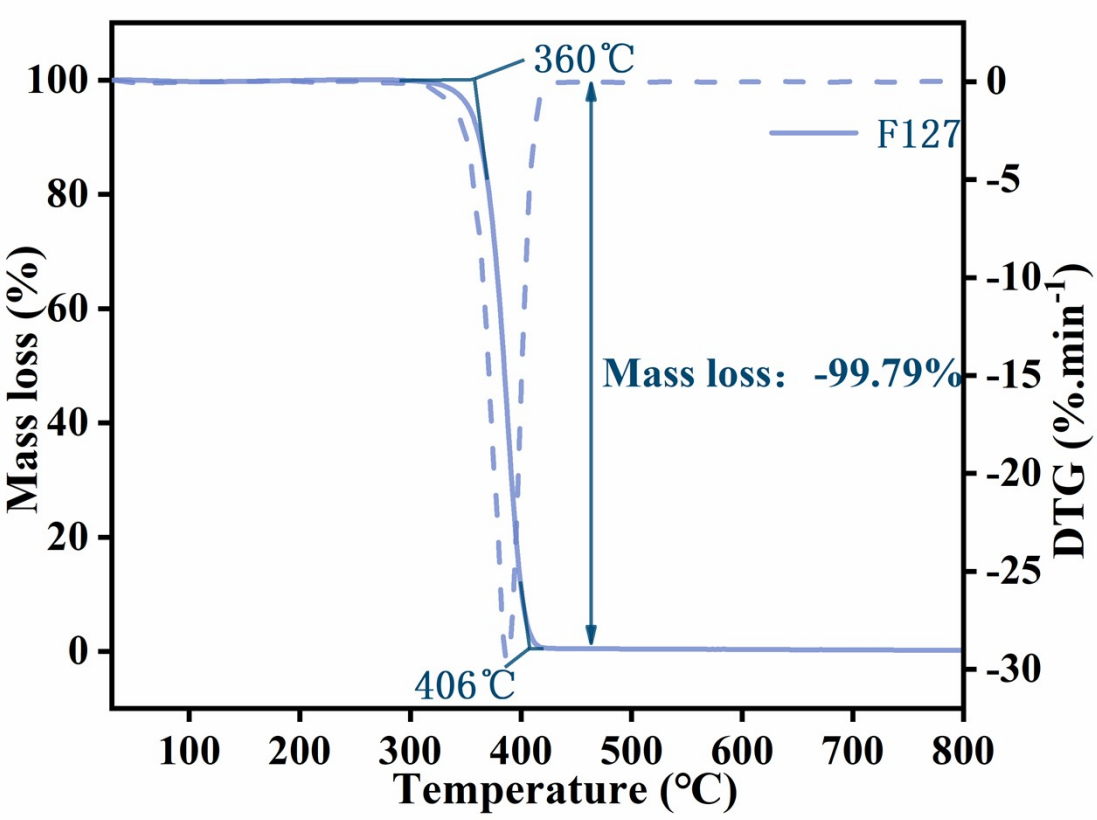


Figure S6 TGA curve of F127. The solid line and dashed line represent the curve of mass loss and DTG with temperature, respectively.

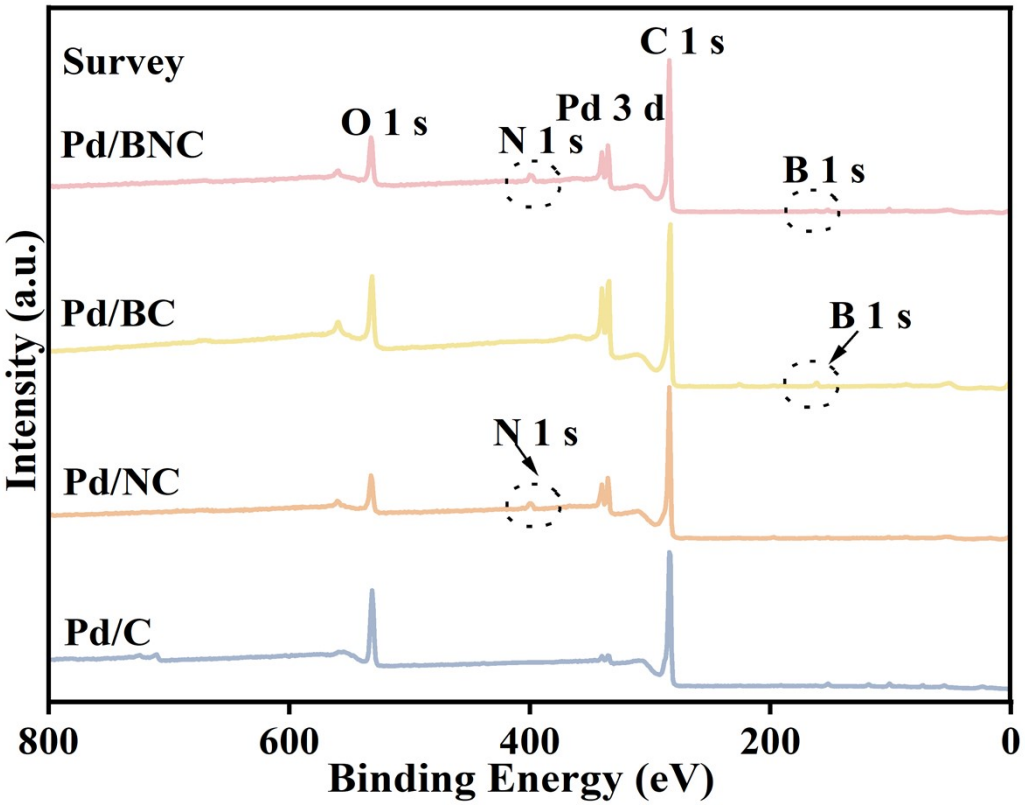


Figure S7 XPS survey spectra of Pd/C, Pd/NC, Pd/BC, and Pd/BNC.

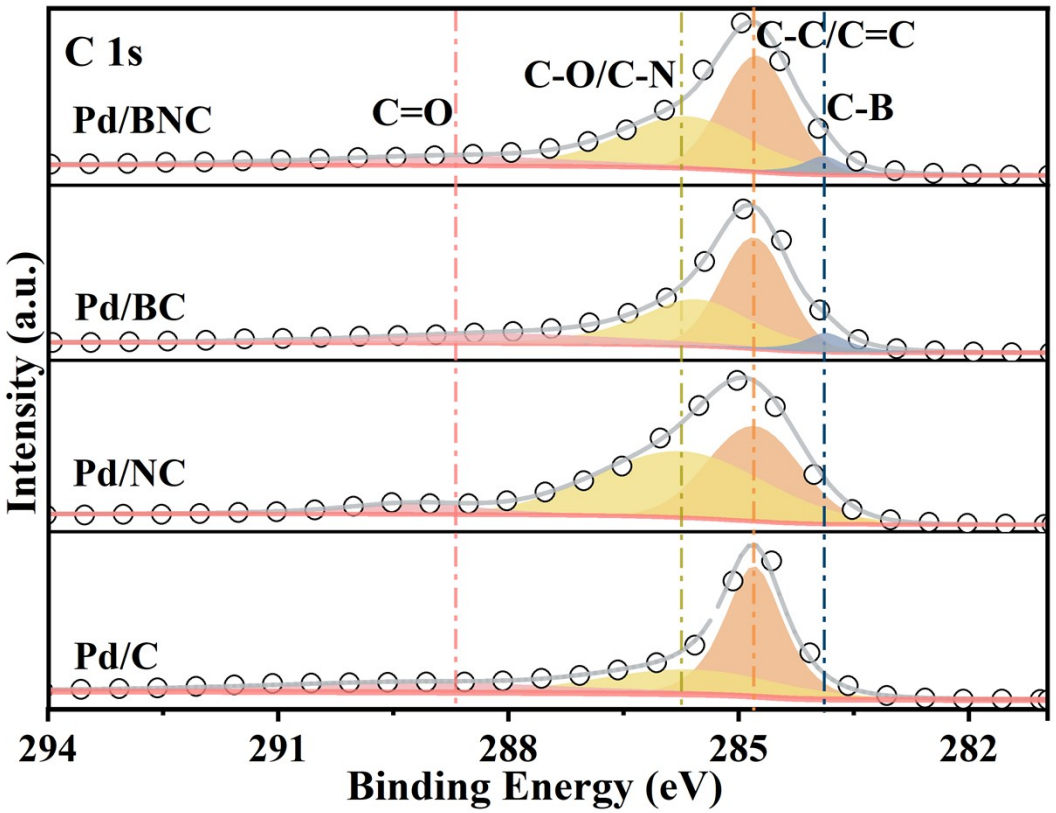


Figure S8 The high-resolution XPS spectra of C 1s in Pd/C, Pd/BC, Pd/NC, and Pd/BNC.

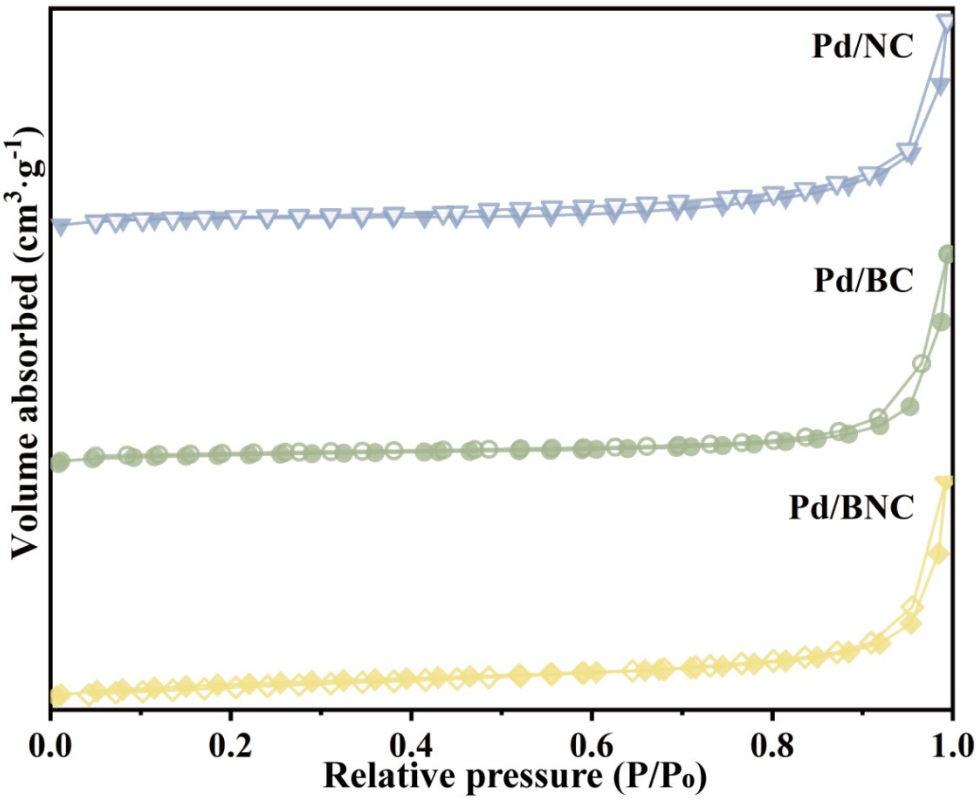


Figure S9 N_2 adsorption-desorption isotherms at 77K of Pd/NC, Pd/BC, and Pd/BNC.

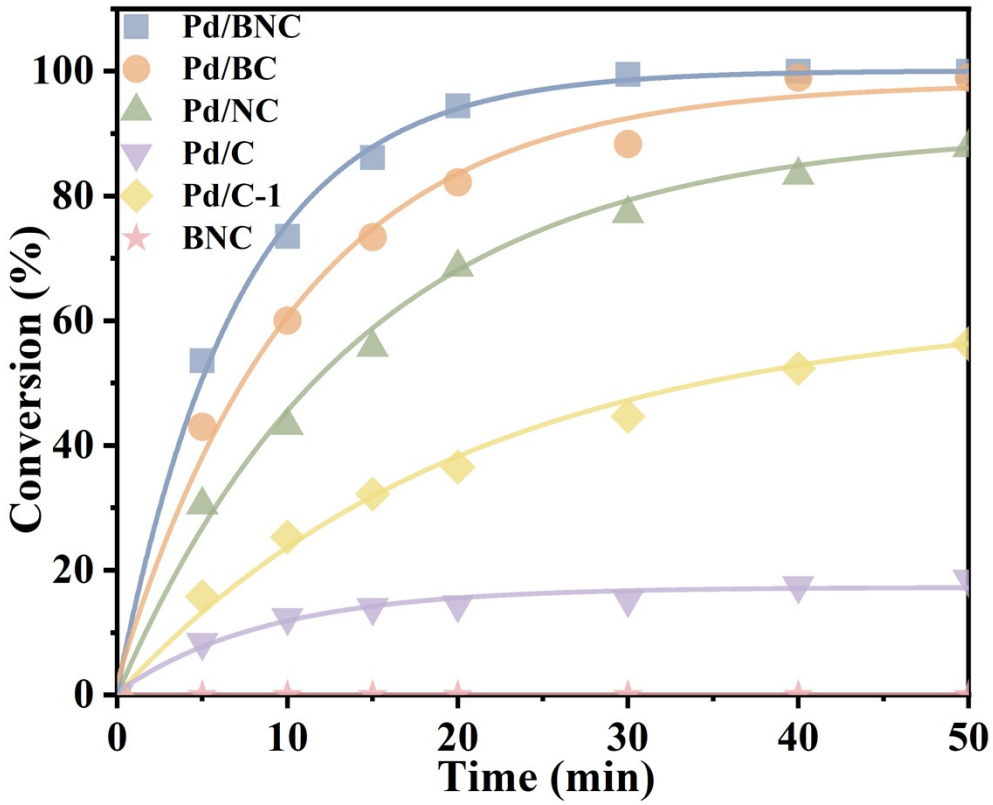


Figure S10 4-CP transformation (%) versus time (min) on the HDC for BNC, Pd/C, Pd/C-1, Pd/NC, Pd/BC, and Pd/BNC catalyst (a). Reaction conditions: catalyst: 0.01g, 4-CP: 5mL ($C_{4\text{-CP}}$: 4 mg/mL), Hydrogen source HCOOH/HCOONa:10 mL (HCOOH: 0.8 mol/L with HCOONa: 1 mol/L), temperature = 40 ℃, stirring rate = 1000 rpm.

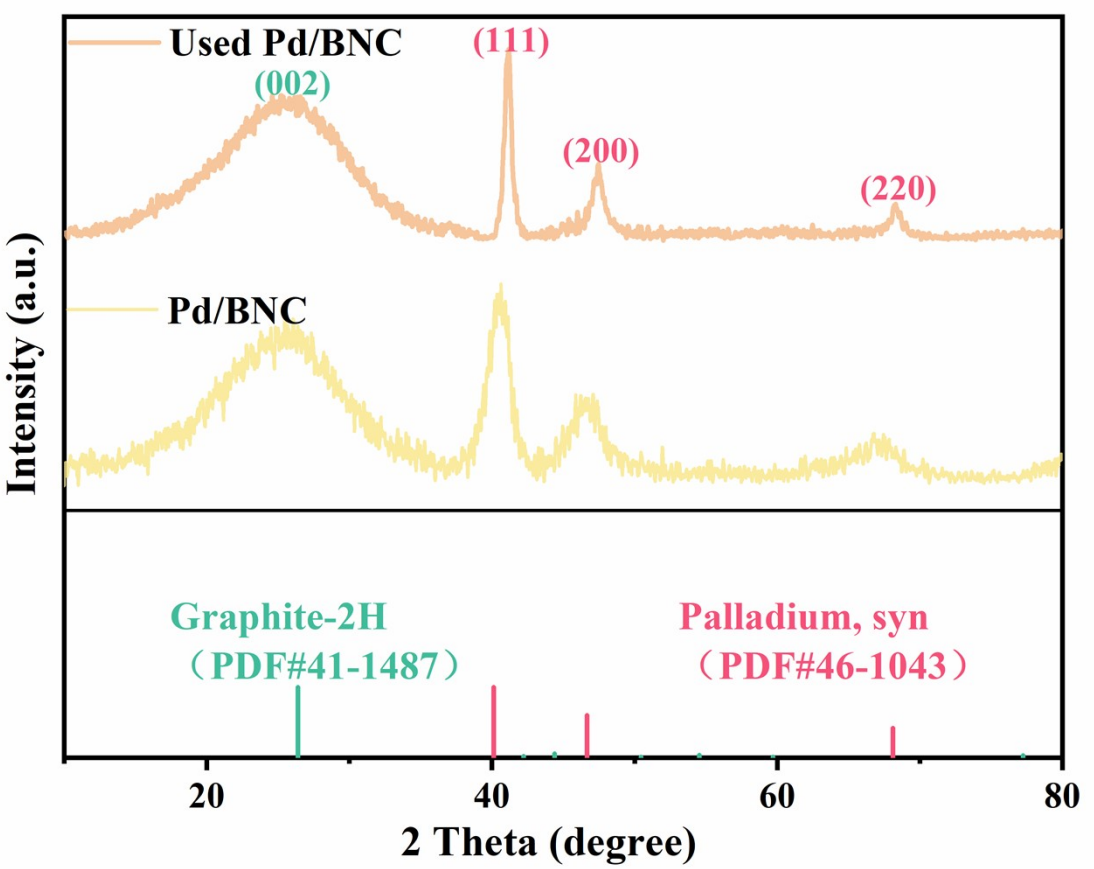


Figure S11 Structural characterizations of used Pd/BNC catalyst. X-ray powder diffraction patterns for the catalyst before and after 10 cycles used.

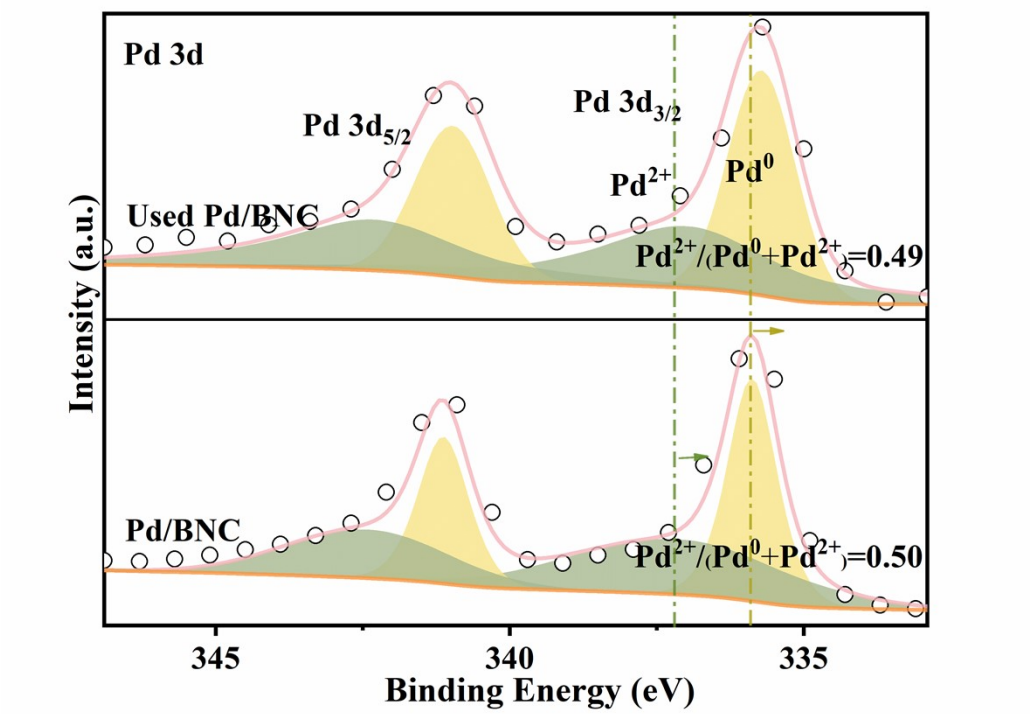


Figure S12 XPS Pd 3d spectra of used Pd/BNC catalyst for 10 run times.

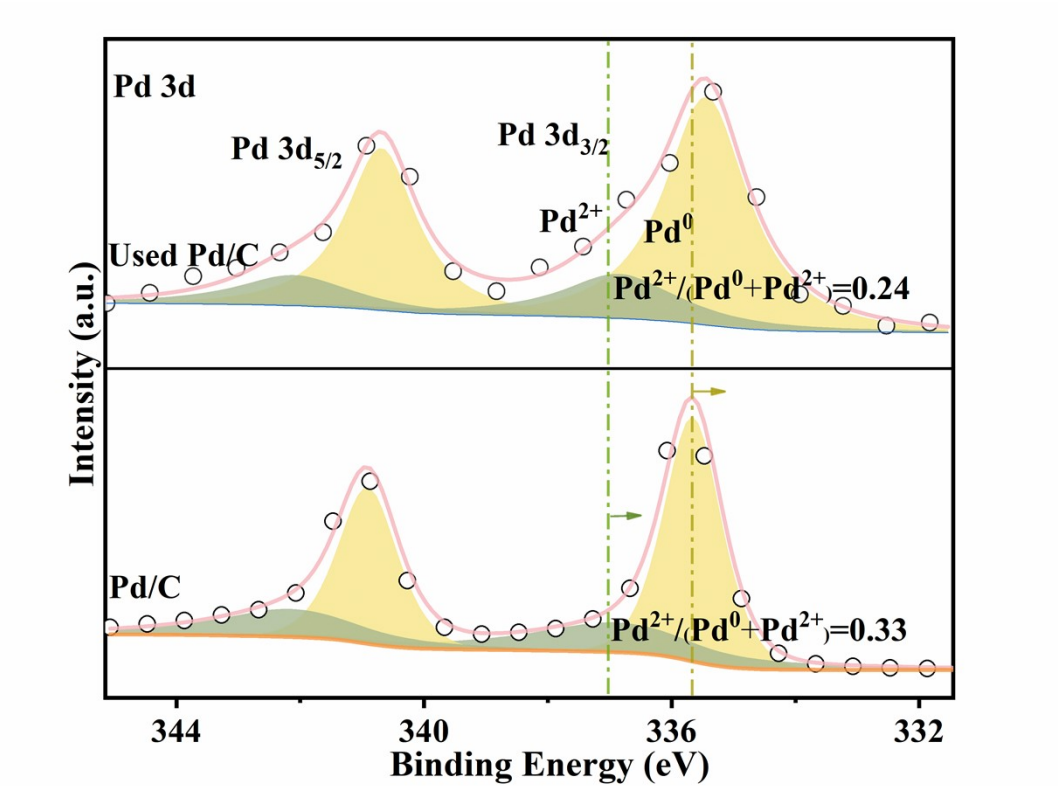


Figure S13 XPS Pd 3d spectra of used Pd/C catalyst for 10 run times.

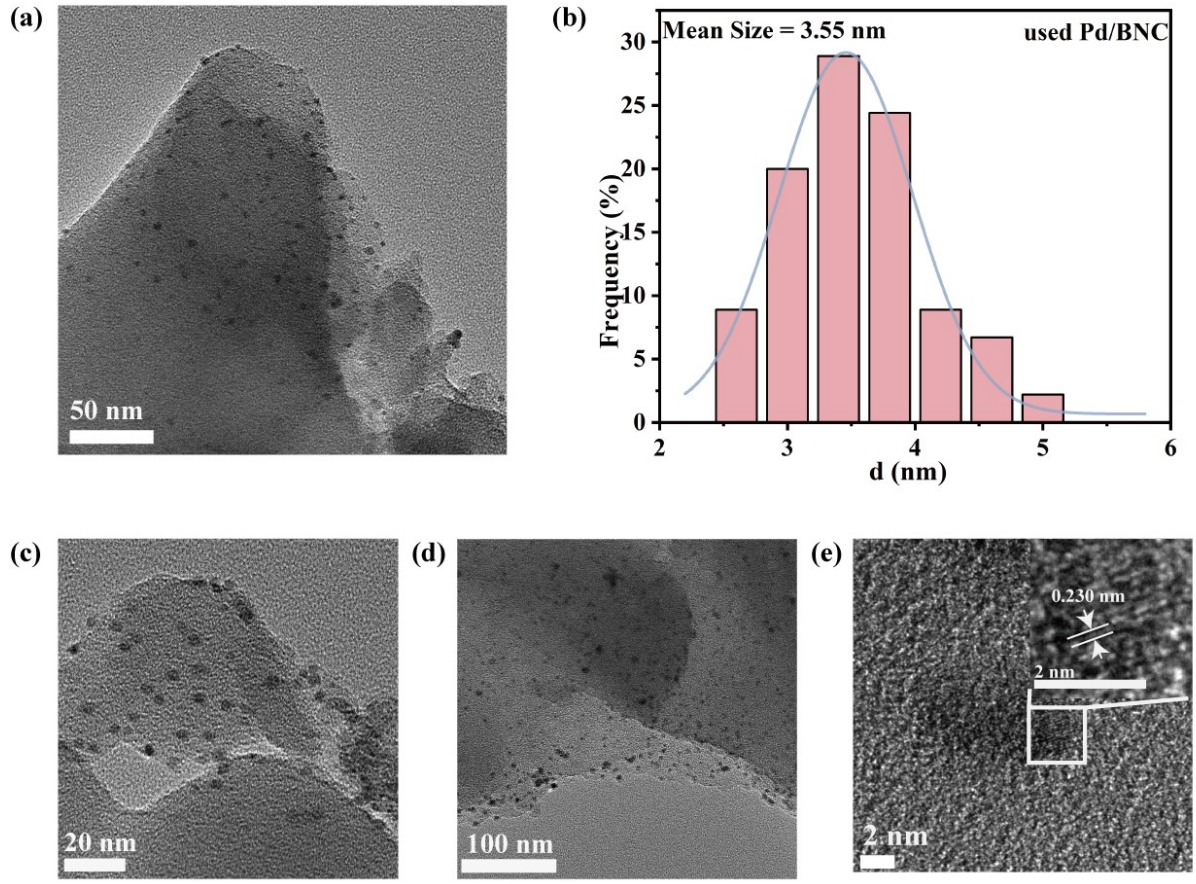


Figure S14 TEM image with scale around 50 nm (a), 20 nm (c), and 100 nm (d), the corresponding particle size distribution with scale around 50 nm (b), and HAADF-STEM images of used Pd/BNC catalyst for 10 run times (e).

Table S1. Pd NPs size values of these Pd/C, Pd/BC, Pd/NC, Pd/BNC using the Sherrer equation.

Sample	Pd/C	Pd/NC	Pd/BC	Pd/BNC
Pd NPs size/nm	8.2	4.2	3.7	3.5

Table S2 The surface and bulk contents of N, B, Pd in Pd/C, Pd/C-1, Pd/NC, Pd/BC, Pd/BNC.

Samples	N (w%)		B (w%)		Pd (w%)	
	Bulk	Surface	Bulk	Surface	Bulk	Surface
Pd/C	——	——	——	——	4.98	5.62
Pd/C-1	——	——	——	——	4.98	4.79
Pd/NC	4.74	4.60	——	——	5.00	4.75
Pd/BC	——	——	3.37	3.16	5.01	4.71
Pd/BNC	4.96	4.70	3.40	3.31	4.99	4.82

Table S3. Specific Surface Area and Pore Structure Results of synthesized carbon materials.

Sample	$S_{BET}/m^2 \cdot g^{-1}$	$S_{mic}/m^2 \cdot g^{-1}$	$V/cm^3 \cdot g^{-1}$	$V_{mic}/cm^3 \cdot g^{-1}$
Pd/C	408	179	0.495	0.392
Pd/NC	336	119	0.221	0.196
Pd/BC	207	132	0.243	0.162
Pd/BNC	277	123	0.215	0.179

Table S4 Values of the first-order rate constants of Figure 7a for HDC of 4-CP.

Sample	k/min^{-1}
Pd/C	-0.007
Pd/C-1	-0.023
Pd/NC	-0.055
Pd/BC	-0.084
Pd/BNC	-0.140