Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information

A Comparative Study of Nitrobenzene Reduction using model catalysts

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Experimental

Materials: Phenanthraquinone (99%), phthalide (98%) and nitrobenzene (99%) were purchased from Alfa Aesar. 9, 10-anthraquinone (98%), benzyl benzoate (GR) and benzyl ether (97%) were bought from Aladdin Reagent Co. Ltd., Shanghai, China. Hydrazine monohydrate (85%), terephthalic acid (99%), ethanol (AR) and other solvents (AR) were supplied by China Medicine Group Shanghai Chemical Reagent Company.

Catalytic reactions: Typically, a certain amount of catalyst, 1.2 g of nitrobenzene, 6.0 equivalent of hydrazine monohydrate and 2 mL of ethanol were charged into a 25 mL round-bottom flask. The flask was then immersed in an oil bath and heated under a water-cooled condenser and kept for a period of time. The reaction temperature here was the temperature of the oil bath. When the reaction was finished, methanol/water (volume ratio 75:25) was added and the mixture was diluted exactly to 50 mL in a volumetric flask. The products were analyzed by HPLC (Elite, UV detector, mobile phase: 75/25 (v/v) methanol/water) with SinoChrom ODS-BP column.

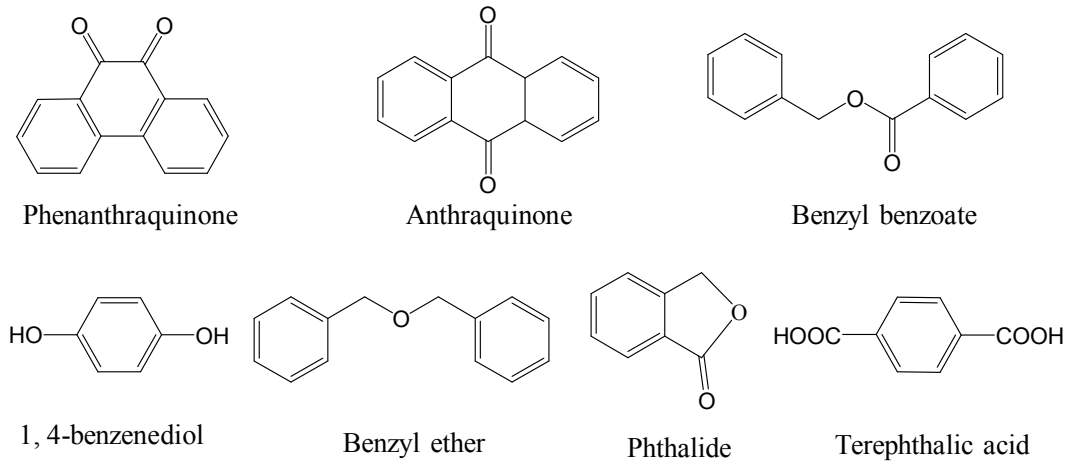

Figure S1. Structure of the catalyst and each additive

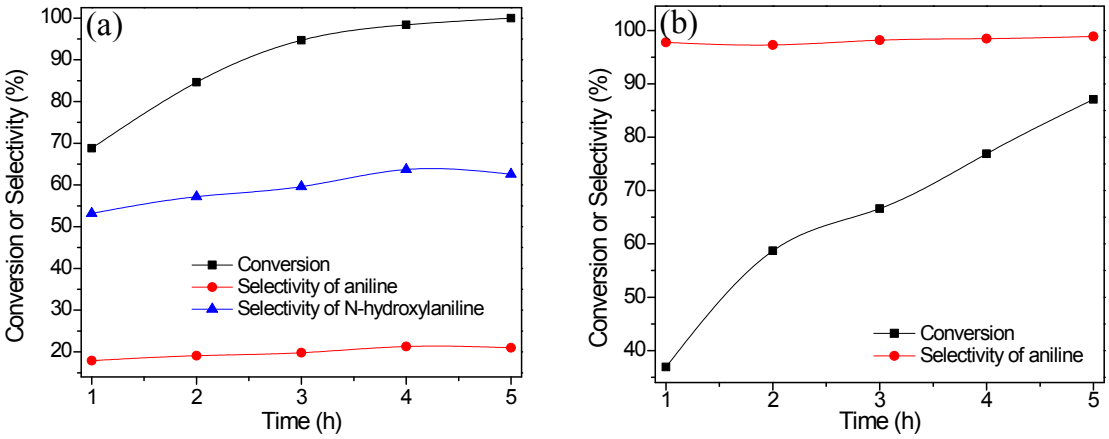

Figure S2. PQ and AQ catalyzed reduction of nitrobenzene at 90 °C
Reaction condition: 30 mg of catalyst, 1.2 g of nitrobenzene, 6.0 equivalent of hydrazine hydrate, 2 mL of ethanol, 90°C.

Table S1. Reduction of nitrobenzene in different solvents

Solvent	Conv. (%)	Sel. (aniline, %)	Y. (aniline, %)
Ethanol	93.4	42.1	39.3
Methanol	86.6	43.4	37.6
Water	70.1	61.9	43.4
THF	32.2	24.5	7.9
Chloroform	10.2	12.0	1.2
Acetone	60.4	42.7	25.8
Acetonitrile	82.2	36.9	30.3
Dioxane	79.6	40.8	32.5
Benzotrifluoride	69.3	53.1	36.8

Reaction condition: 15 mg of phenanthraquinone, 1.2 g of nitrobenzene, 6.0 equivalent of hydrazine hydrate, 2 mL of solvent, 100^{o}C, 3 h.

Table S2. Reduction of nitrobenzene in different solvents

Solvent	Conv. (%)	Sel. (aniline, %)	Y. (aniline, %)
Ethanol	80.4	75.1	60.4
Methanol	75.2	76.8	57.8
Water	58.1	89.9	52.2
THF	26.7	51.3	13.7
Chloroform	9.6	14.4	1.4
Acetone	54.1	76.5	41.4
Acetonitrile	73.7	67.1	49.4
Dioxane	71.8	70.7	50.8
Benzotrifluoride	60.5	83.3	50.4

Reaction condition: 5 mg of phenanthraquinone, 1.2 g of nitrobenzene, 6.0 equivalent of hydrazine hydrate, 2 mL of solvent, 100^{o}C, 3 h.