Efficient Catalytic Oxidation of Methyl Aromatic Hydrocarbon with N-Alkyl Pyridinium Salts

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Supplementary Material

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Correlative FT-IR and NMR spectrums:

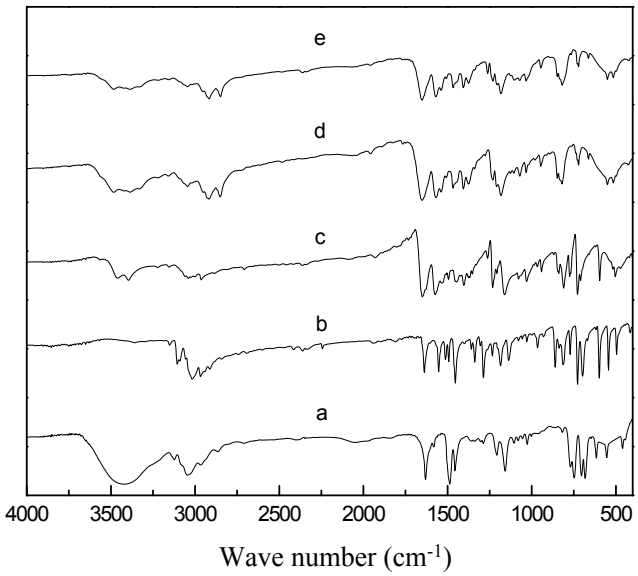
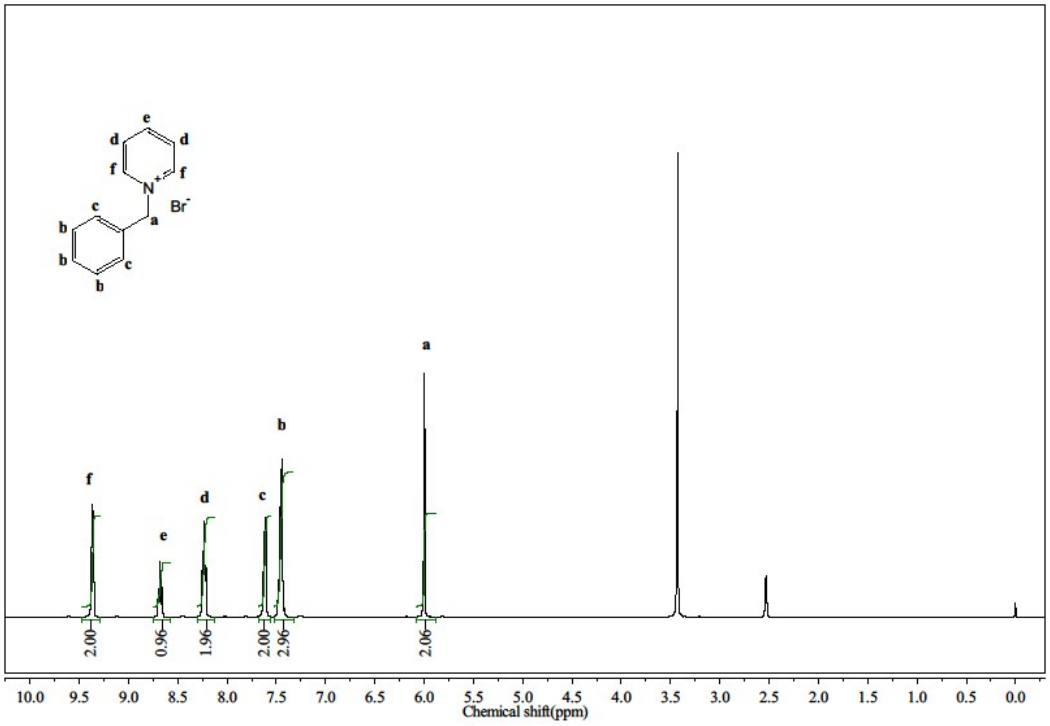
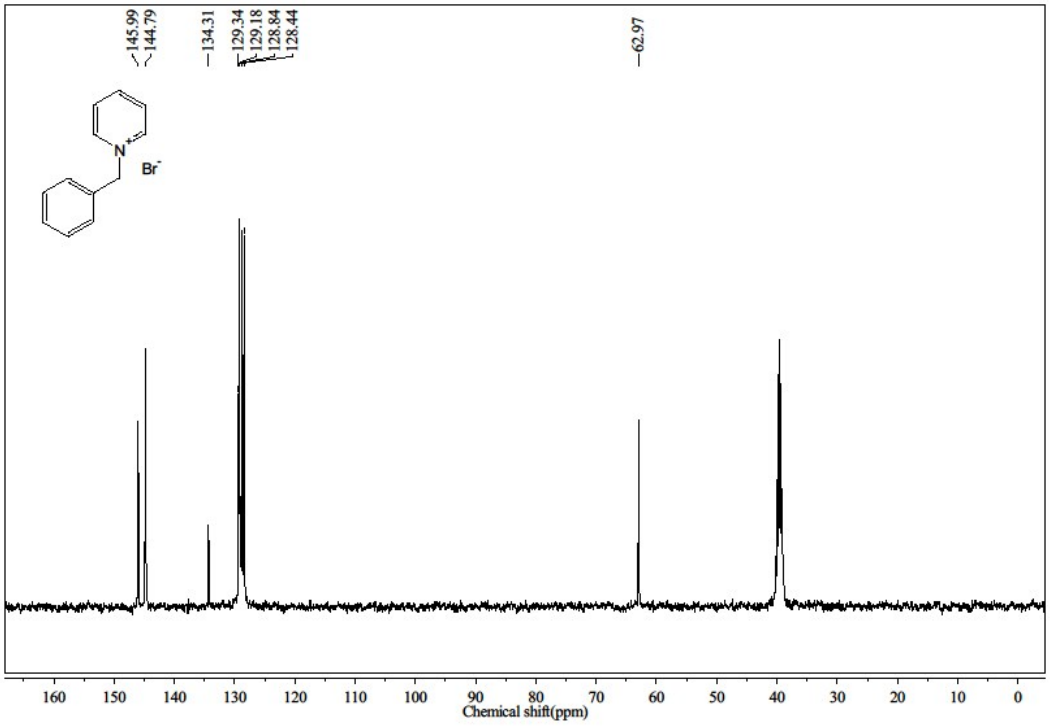


Figure S1. FT-IR spectrum for different *N*-alkylpyridinium salt.

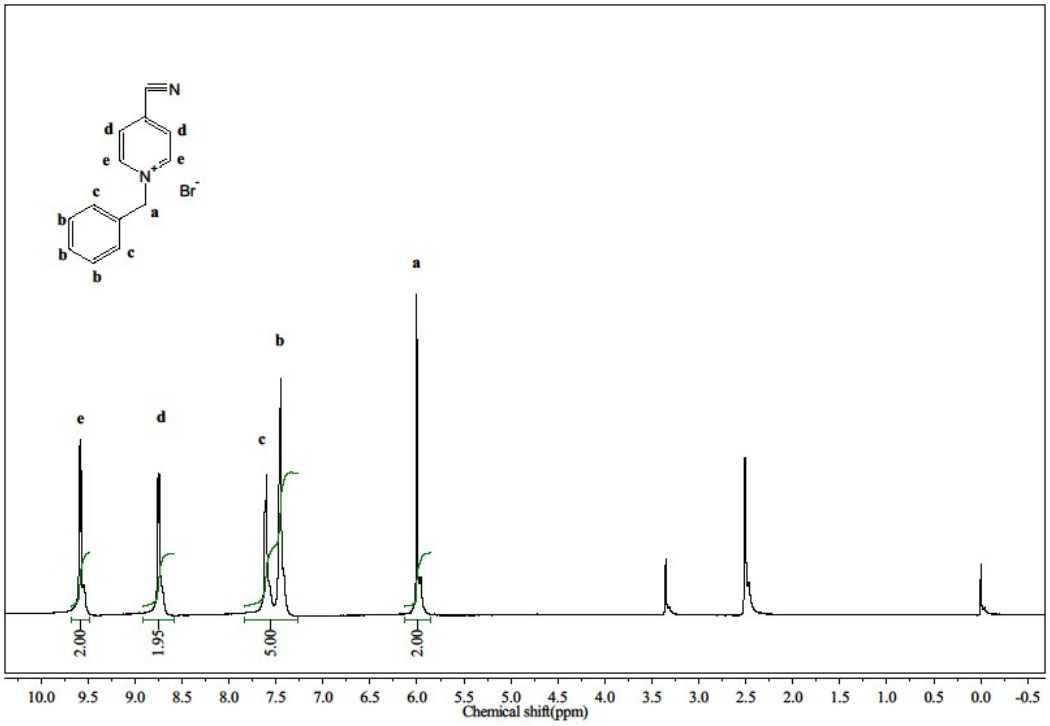


a. ^{1}H NMR spectrum

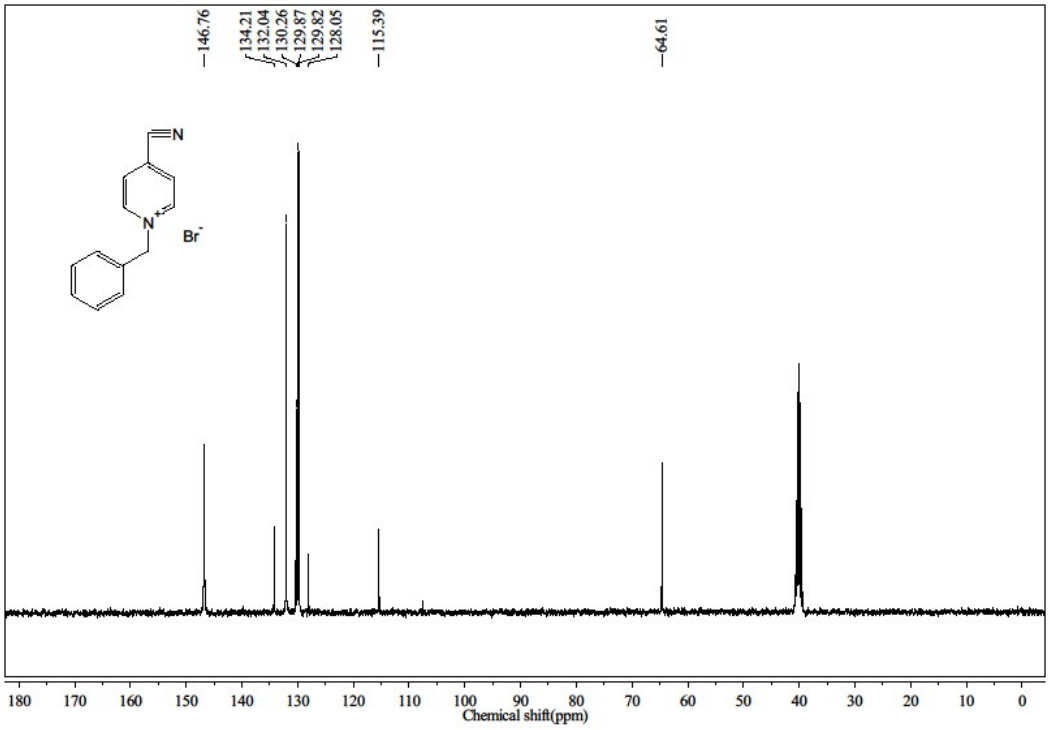


b. ^{13}C NMR spectrum

Figure S2. NMR spectrum of 1-benzyl pyridinium bromide.

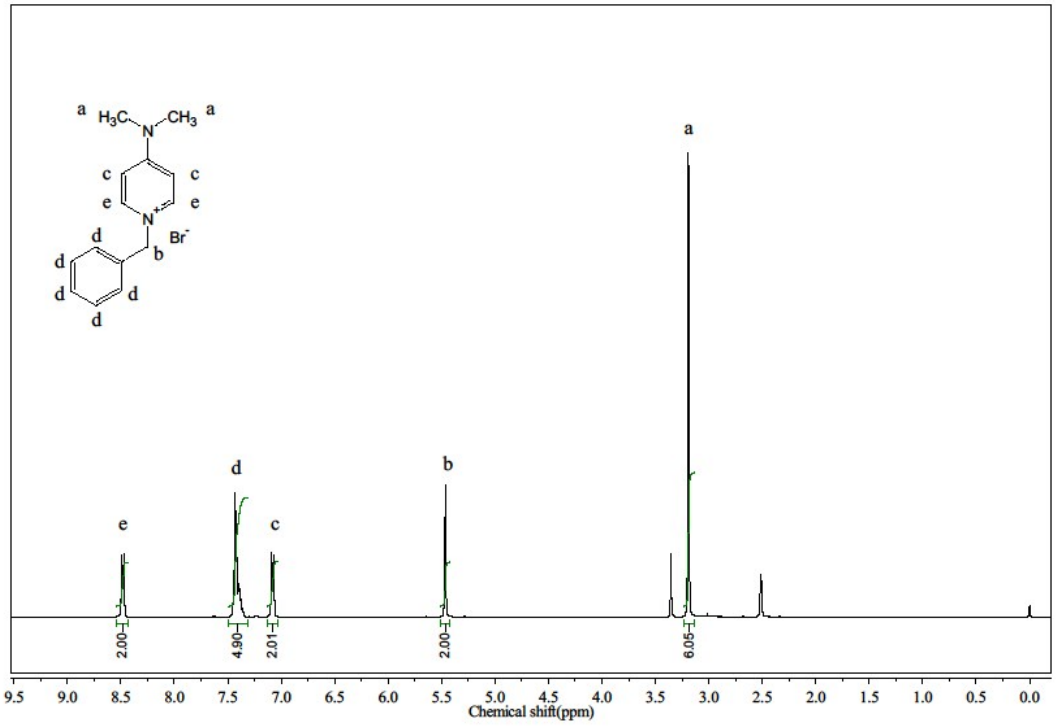


a. ^{1}H NMR spectrum

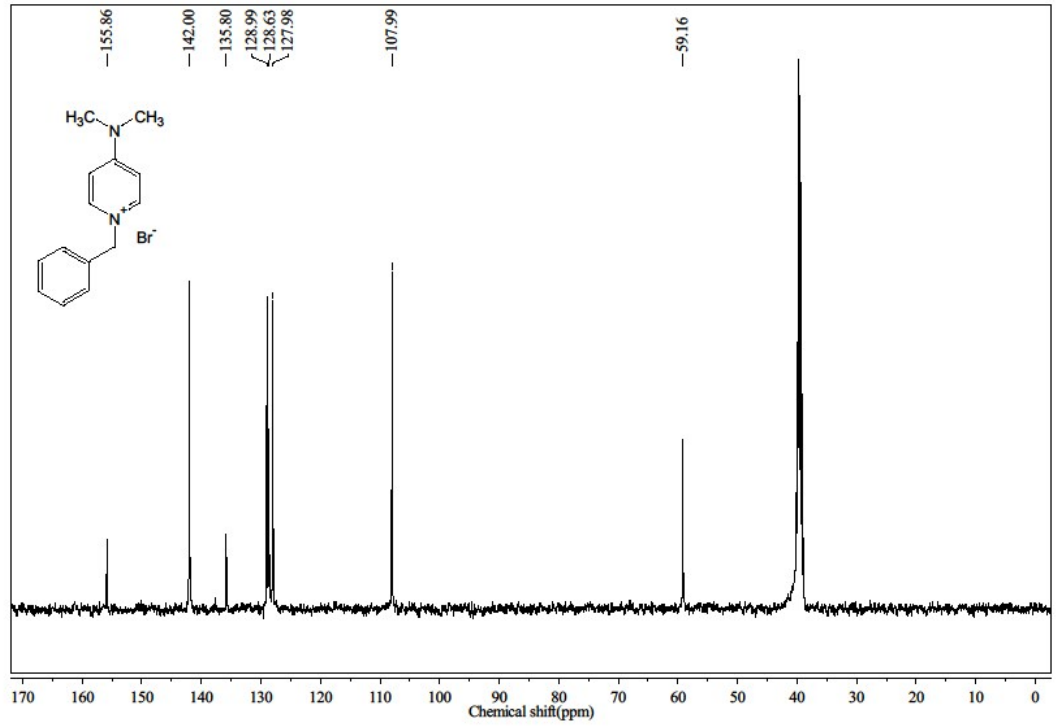


b. ^{13}C NMR spectrum

Figure S3. NMR spectrum of 1-benzyl-4-cyano pyridinium bromide.

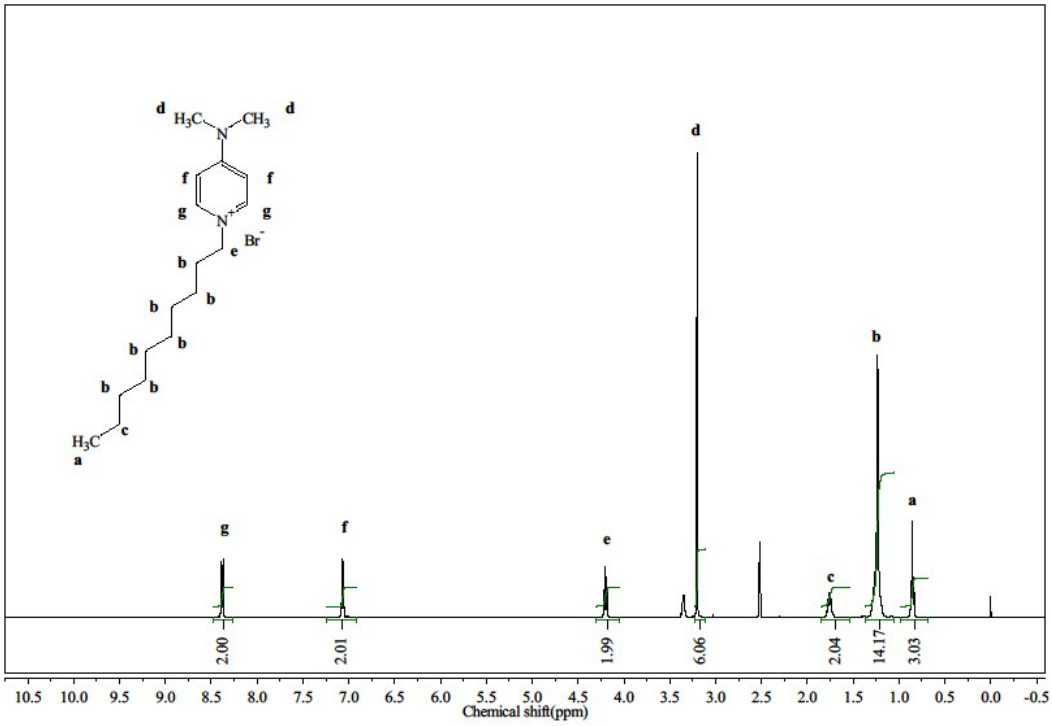


a. ^{1}H NMR spectrum

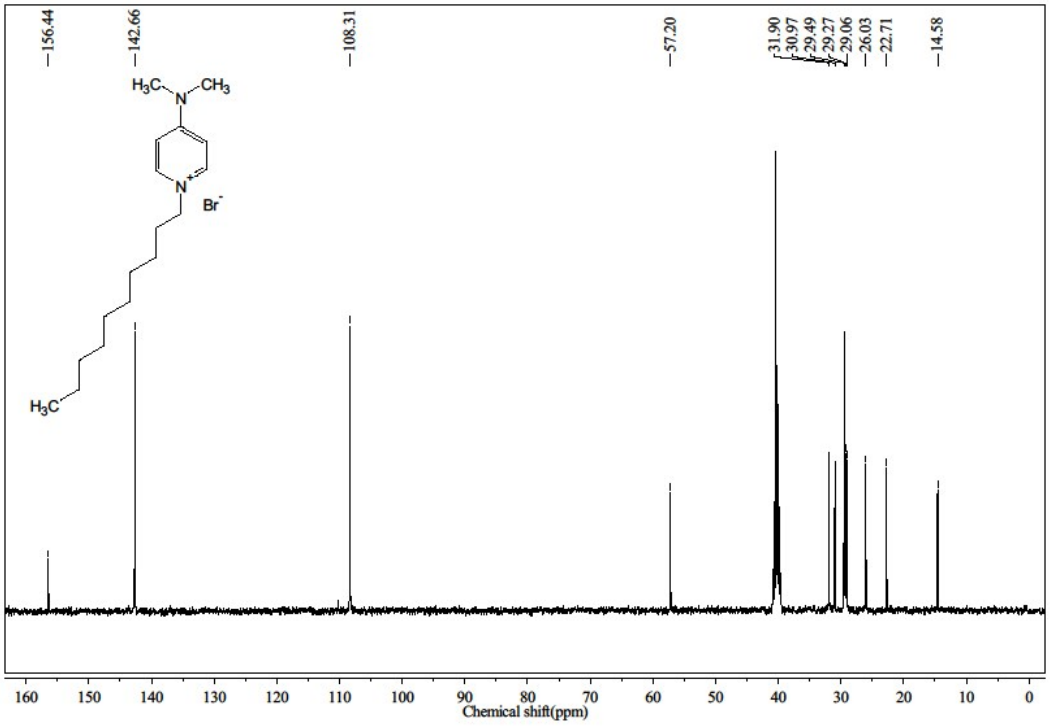


b. ^{13}C NMR spectrum

Figure S4. NMR spectrum of 1-benzyl-4-dimethylaminopyridinium bromide.

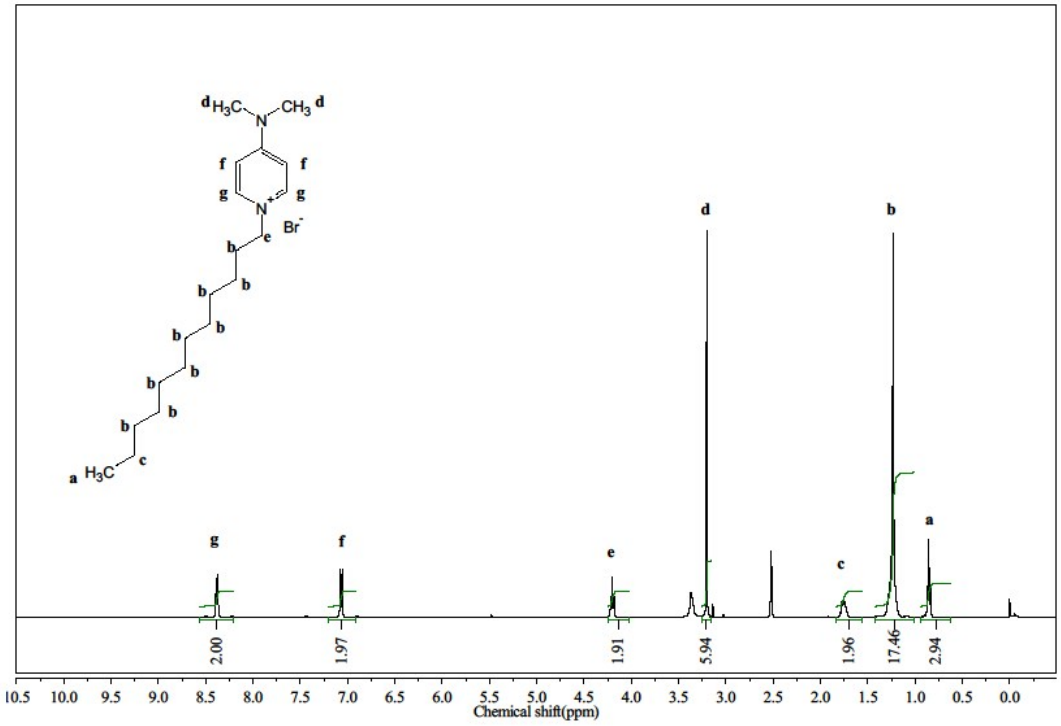


a. ^{1}H NMR spectrum

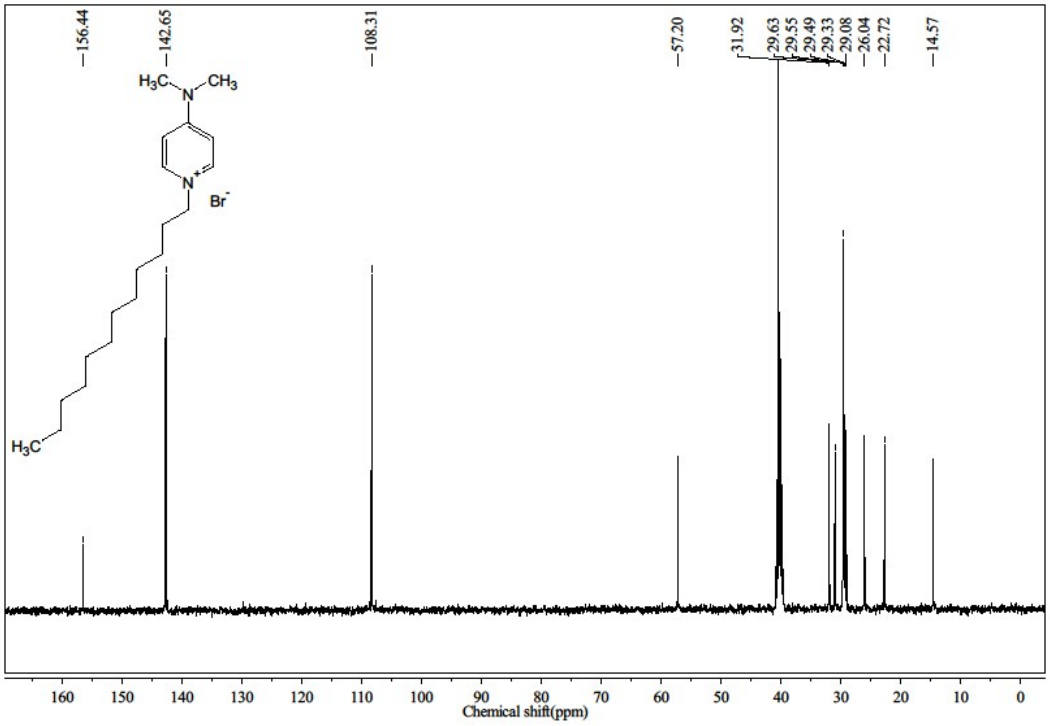


b. ^{13}C NMR spectrum

Figure S5. NMR spectrum of 1-decyl-4-dimethylaminopyridinium bromide.



a. ^{1}H NMR spectrum



b. ^{13}C NMR spectrum

Figure S6. NMR spectrum of 1-dodecyl-4-dimethylaminopyridinium bromide.

Optimization of reaction temperature

Using **c** as catalyst, the results for *p*-xylene oxidation under different temperature were shown in Figure S7. Increasing the temperature, the conversion of *p*-xylene increased. Further increasing the temperature from 160 ^{o}C to 180 ^{o}C, the *p*-xylene conversion increased little. Optimized reaction temperature was selected as 160 ^{o}C. However, the yield of *p*-toluic acid (TA) decreased, while formation of deep oxidation product of 4-CBA and TPA increased.

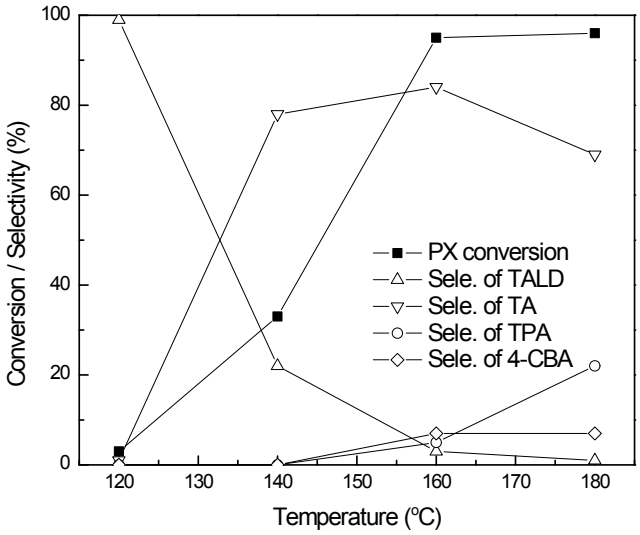


Figure S7. Influence of temperature on the catalytic oxidation of *p*-xylene. Reaction conditions：10 mmol of *p*-xylene, 0.5 mmol of **c**, 5 ml of acetonitrile, 0.2 mmol of *p*-tolualdehyde as initiator, 1.5 MPa O_2, 4h.

Optimization of catalyst concentration

Using **c** as the catalyst, the optimization of different catalyst concentration was also

carried out. The results were shown in Figure S8. When 1 mol % of **c** was used as the catalyst, the conversion of *p*-xylene was 55 %. Increasing the catalyst concentration from 1 mol % to 5 mol %, the *p*-xylene conversion increased to 95 %. Further increasing the catalyst concentration to 7 mol %, however, no remarkable improvement for the oxidation was observed. Therefore, the catalyst concentration of 5 mol % was suitable.

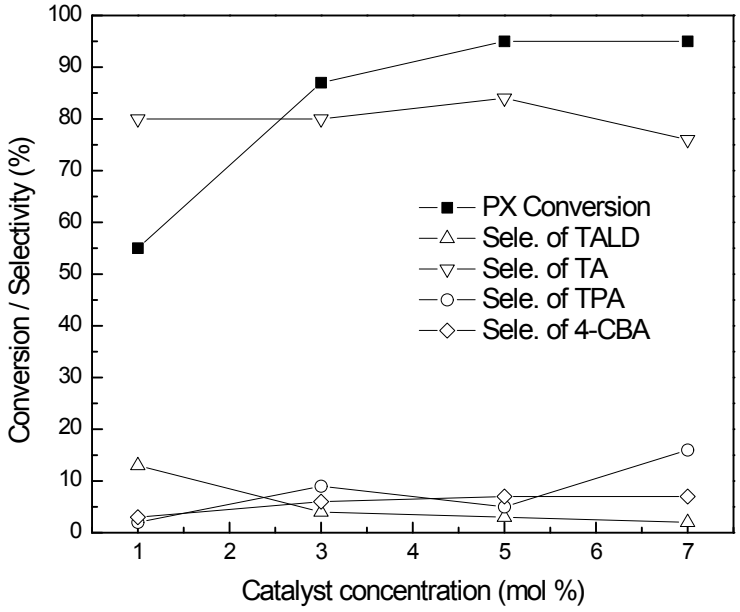


Figure S8. The effect of catalyst concentration

Reaction conditions：10 mmol of *p*-xylene, 5 ml of acetonitrile, 0.2 mmol of *p*-tolualdehyde as initiator, **c** used as catalyst, 1.5 MPa O_2, 160 ^oC, 4h.