

Supporting Information

AlBr₃·6H₂O Catalyzed Oxidation of Alcohols

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General information

$\text{AlBr}_3 \cdot 6\text{H}_2\text{O}$ was obtained from commercial sources. All solvents used were analytical grade and were used as received. All of the alcohols used in the reaction were obtained from ABCR GmbH & Co. KG. and used as received without further treatment. H_2^{18}O was obtained from Huayi Isotope Co. and used as received. All NMR spectra are recorded on MERCURY (400 MHz for ^1H NMR, 100 MHz for ^{13}C NMR) spectrometers; chemical shifts are expressed in ppm (δ units) relative to TMS signal as internal reference in CDCl_3 . Gas chromatography (GC) analysis was performed on a Shimadzu GC-2010 equipped with a $15\text{ m} \times 0.53\text{ mm} \times 1.5\text{ }\mu\text{m}$ RTX-1 capillary column and a oxyhydrogen flame detector. GC/MS analysis were carried out on a trace HP GC6890/MS5973 equipped with a $25\text{ m} \times 0.25\text{ mm}$ SE-54 column and a Shimadzu GC-16A gas chromatograph with a $3\text{ m} \times 3\text{ mm}$ OV-17 column.

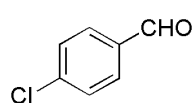
General procedure for the oxidation of alcohols with $\text{AlBr}_3 \cdot 6\text{H}_2\text{O}$

To a 10 mL round flask were added 0.10 mmol alcohol substrate, 2 mL of 1, 4-dioxane, and 0.03 mmol $\text{AlBr}_3 \cdot 6\text{H}_2\text{O}$ (0.011 g). Then the flask was immersed in a preheated $70\text{ }^\circ\text{C}$ oil bath for for the desired reaction time. Percentage conversion and reaction selectivity were determined by GC analysis. The yield was calculated on the basis of 1.0 mmol of substrate. Isolated product is obtained by column chromatograph. (Petroleum ether / ethyl acetate = 1 ~ 10:1)

Preparation of ^{18}O enriched benzyl alcohol

0.05 g Na was added to 0.75 mL ^{18}O enriched water (98 % H_2^{18}O , Huayi Isotope Co.) in a flask, and then 0.5 mL 1-chloromethylbenzene was added into the flask. The mixture was heated to 368 K and refluxed for 48 h with continuous stirring. The product was purified by column chromatography and 0.2 g $\text{C}_6\text{H}_5\text{CH}_2^{18}\text{OH}$ was obtained. The ^{18}O enriched benzyl alcohol was examined by GC-MS, and the abundance of $\text{C}_6\text{H}_5\text{CH}_2^{18}\text{OH}$ was 98 %.

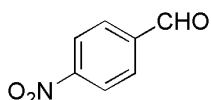
The Data for Products 2b, 3b, 8b, 9b, 9c, 10b, 11b



4-Chlorobenzaldehyde (2b)

^1H NMR (CDCl_3 , 400 MHz): δ = 10.00 (s, 1H, CHO), 7.85 - 7.83 (d, J = 8 Hz, 2H, Ar-H), 7.54 - 7.52 (d, J = 8 Hz, 2H, Ar-H);

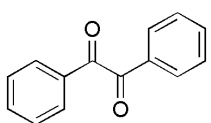
^{13}C NMR (100 MHz): δ = 190.84, 140.92, 134.67, 130.88, 129.42.



4-Nitrobenzaldehyde (3b)

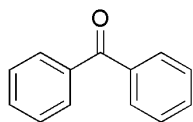
^1H NMR (CDCl_3 , 400 MHz): δ = 10.17 (s, 1H, CHO), 8.42 - 8.40 (d, J = 8 Hz, 2H, Ar-H), 8.10 - 8.08 (d, J = 8 Hz, 2H, Ar-H);

^{13}C NMR (100 MHz): δ = 190.27, 151.10, 140.01, 130.48, 124.31.



Benzil (8b)

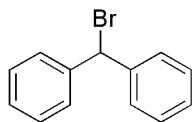
^1H NMR (CDCl_3 , 400 MHz): δ = 7.99 - 7.96 (m, 4H, Ar-H), 7.68 - 7.64 (m, 2H, Ar-H), 7.54 - 7.50 (m, 4H, Ar-H); ^{13}C NMR (100 MHz): δ = 194.56, 134.88, 132.96, 129.89, 129.01.



Benzophenone (9b)

^1H NMR (CDCl_3 , 400 MHz): δ = 7.82 - 7.79 (m, 4H, Ar-H), 7.60-7.58 (m, 2H, Ar-H), 7.49 - 7.45 (m, 4H, Ar-H); ^{13}C NMR

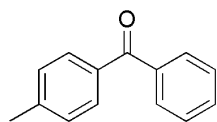
(100 MHz): δ = 196.67, 137.49, 132.35, 129.98, 128.20.



Bromodiphenylmethane (9c)

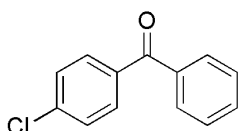
^1H NMR (CDCl_3 , 400 MHz): δ = 7.37 - 7.23 (m, 10H, Ar-H), 5.39 (s, 1H, CH) ; ^{13}C NMR (100 MHz): δ = 142.19, 128.36,

127.41, 127.24, 79.96.



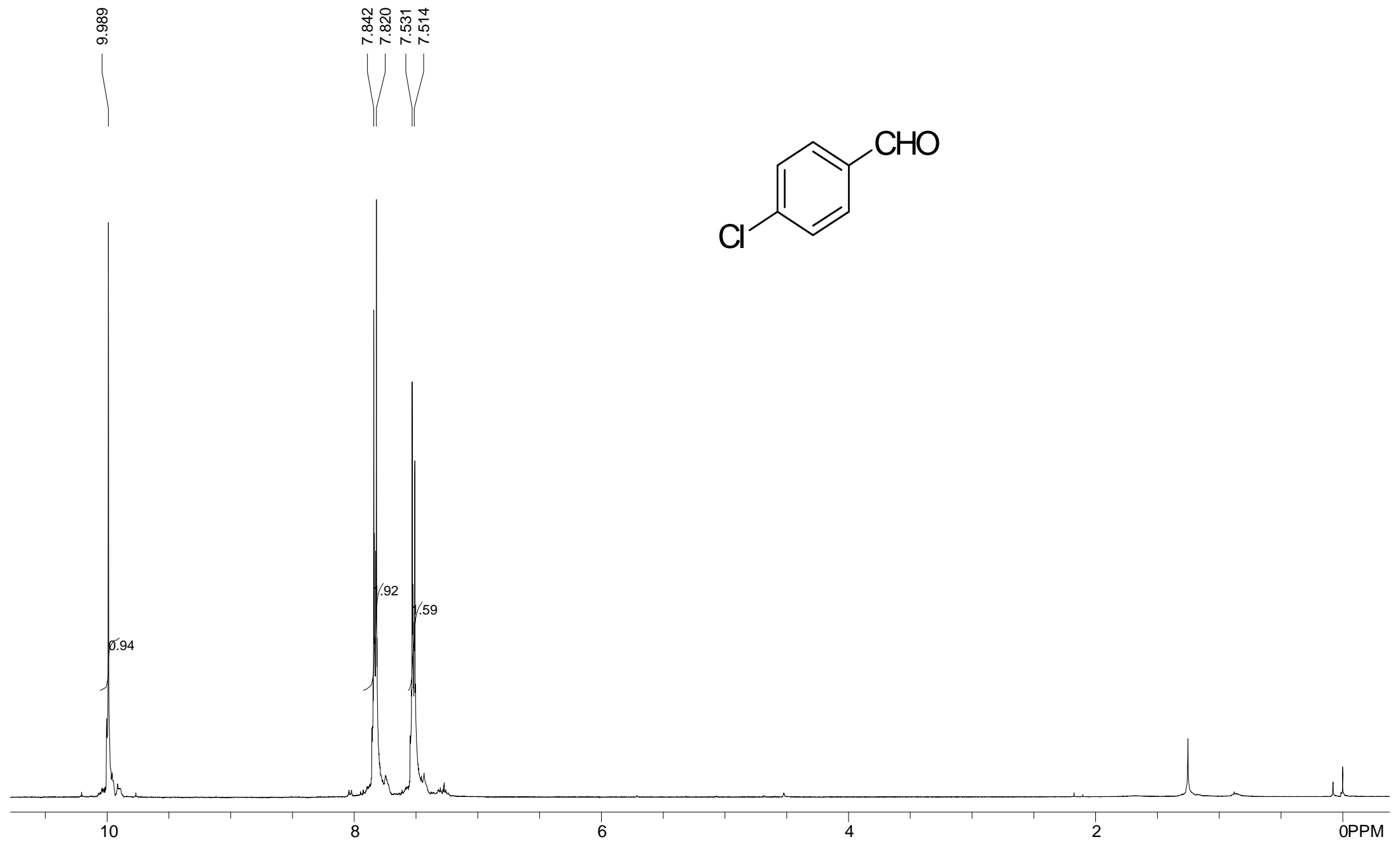
4-Methylbenzophenone (10b)

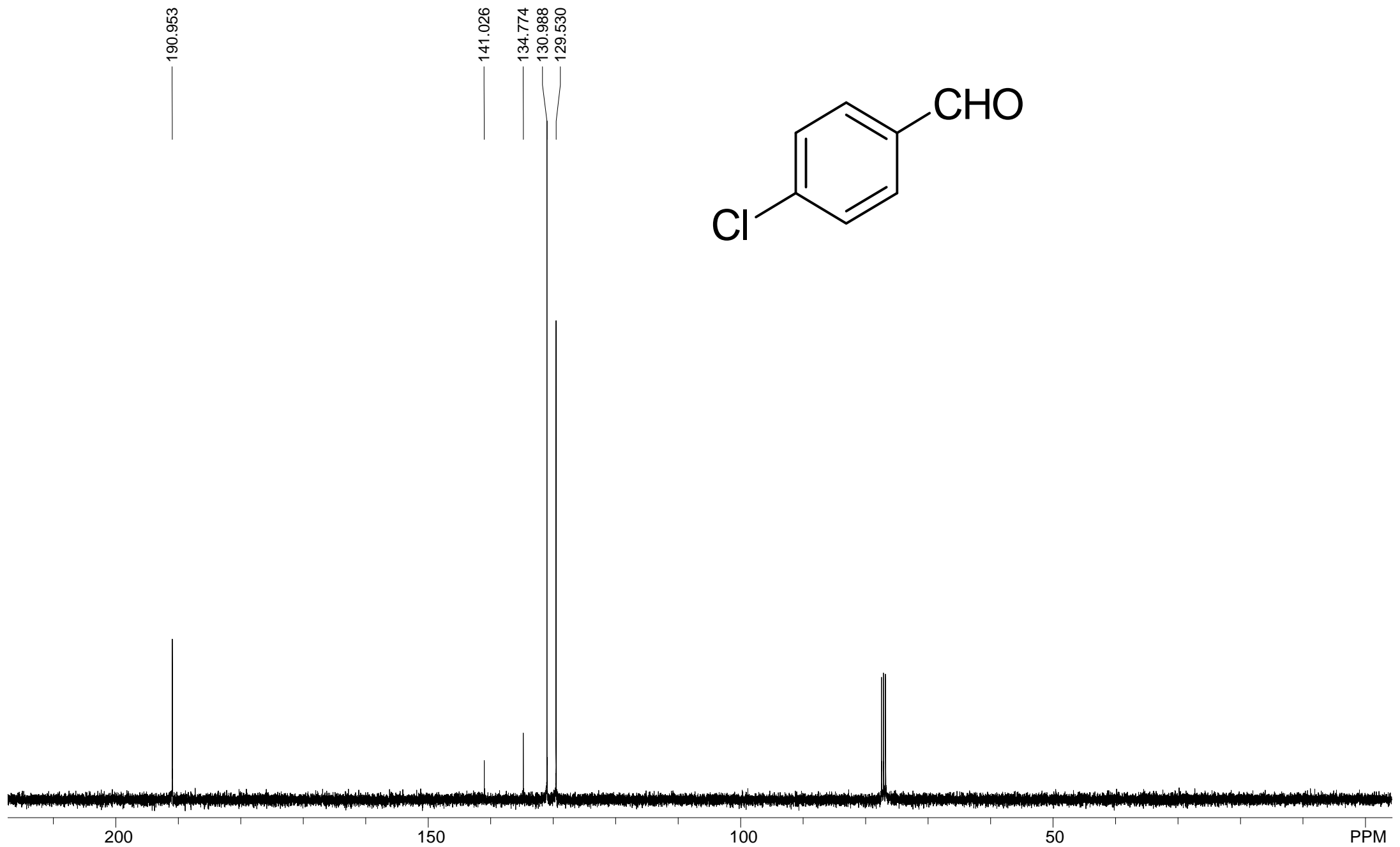
^1H NMR(CDCl_3 , 400 MHz): δ = 7.79 - 7.77 (d, J = 8 Hz, 2H, Ar-H), 7.73 - 7.71 (d, J = 8 Hz, 2H, Ar-H), 7.59 - 7.55 (t, J = 8 Hz, 1H, Ar-H), 7.49 - 7.45 (t, J = 8 Hz, 2H, Ar-H), 7.29 - 7.27 (t, J = 8 Hz, 2H, Ar-H), 2.44 (s, 3H, CH_3); ^{13}C NMR (100 MHz, CDCl_3): δ = 196.43, 143.19, 137.93, 134.87, 132.11, 130.26, 129.88, 128.94, 128.16, 21.63.

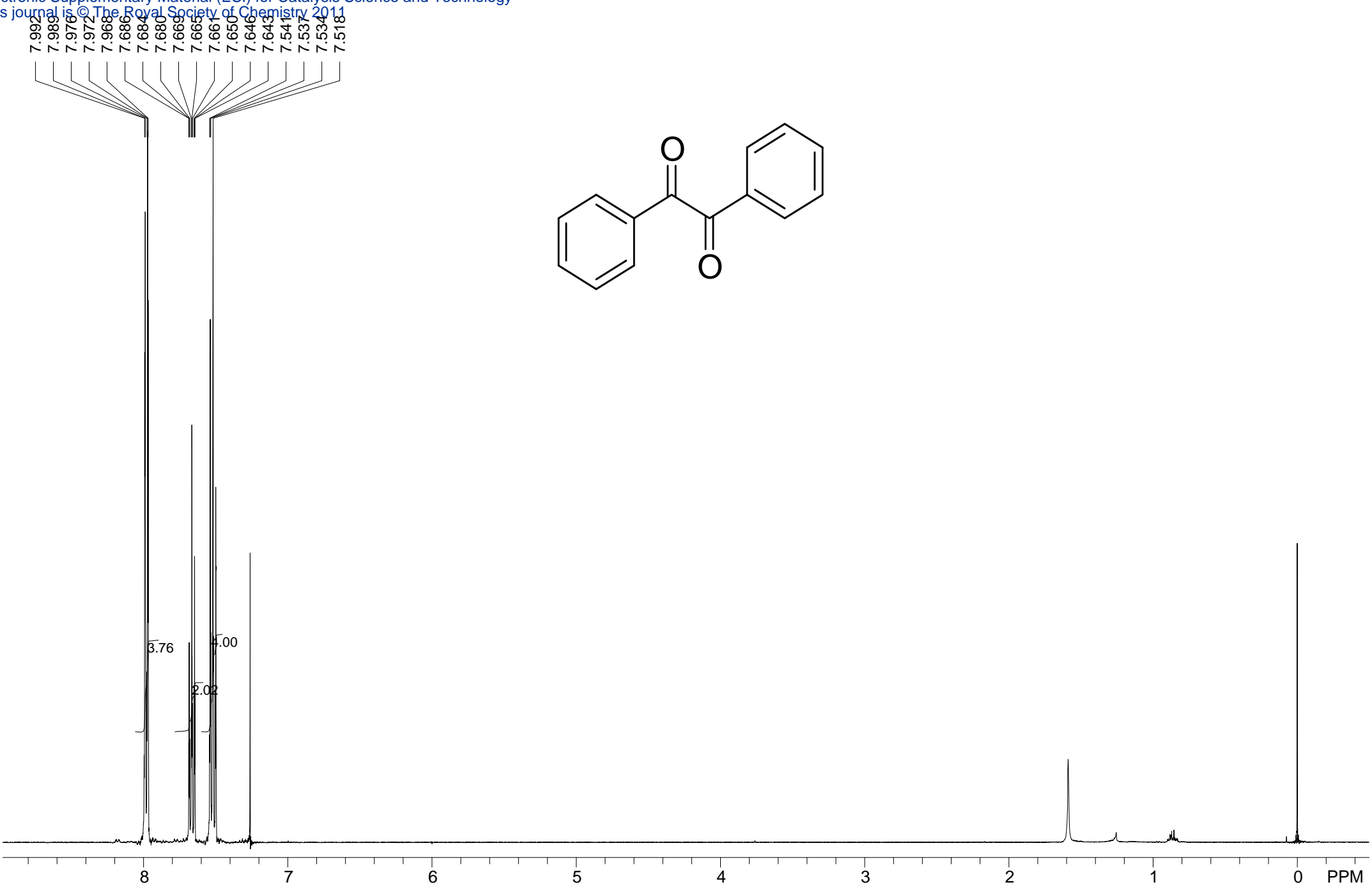
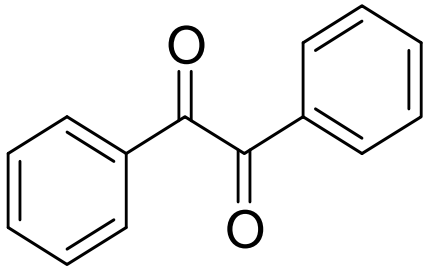


4-Chlorobenzophenone (11b)

^1H NMR (CDCl_3 , 400 MHz): δ = 7.79 - 7.75 (m, 4H, Ar-H), 7.62 - 7.58 (m, 1H, Ar-H), 7.51 - 7.46 (m, 4H, Ar-H); ^{13}C NMR (100 MHz): δ = 195.51, 138.88, 137.21, 135.83, 132.63, 131.45, 129.92, 128.62, 128.39.







194.862
135.179
133.267
130.194
129.306

