Supporting Information

Titanium-based zeolitic imidazolate framework for chemical fixation of carbon dioxide

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1. Synthesis of (2-furan-2-yl)-1*H*-benzo[*d*]imidazole and Ti-ZIF catalyst

a) Synthesis of (2-furan-2-yl)-1*H*-benzo[*d*]imidazole

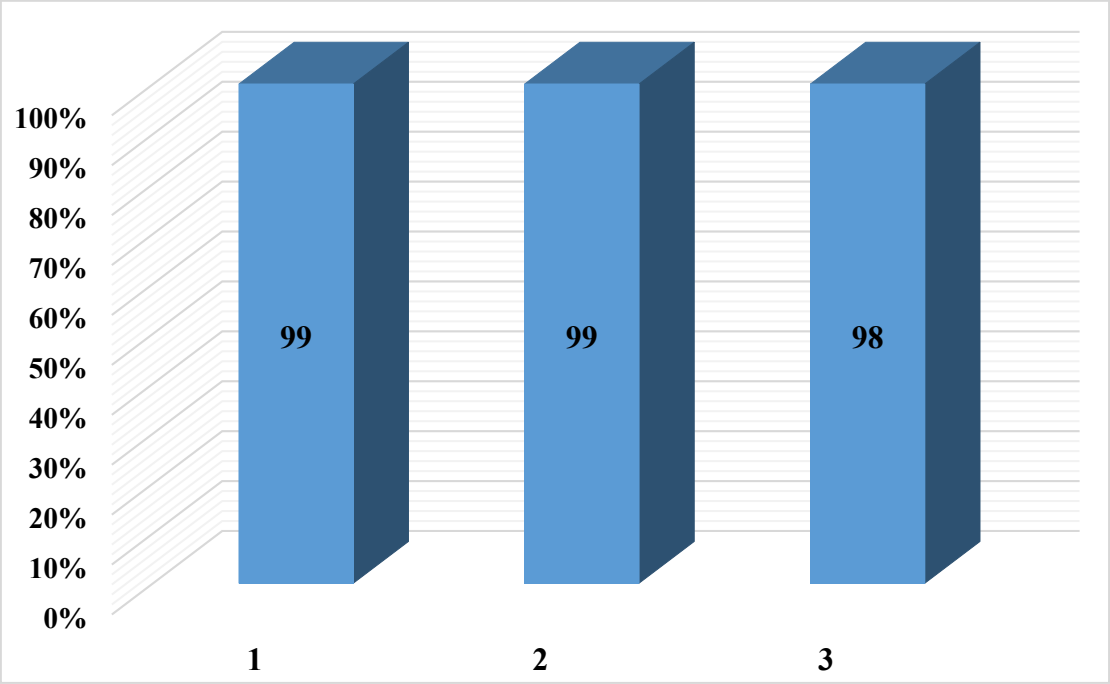
To a mixture of *o*-phenylenediamine (2 mmol; 0.2162 g) and furfural (2 mmol; 0.192 g) in 5 mL of ethanol, 20 mol % of ammonium chloride was added and the solution was stirred at 80 °C. The progress of reaction was monitored by TLC. After completion of the reaction (4.0 hours) the product was extracted using ethyl acetate, dried over sodium sulfate and concentered under reduced pressure. The product was purified using column chromatography (ethyl acetate: hexane, 1:1) and characterized using GC-MS.

b) Synthesis of Ti-ZIF catalyst

Titanium (IV) isobutoxide (4.0 mmol; 1.361 g), (2-furan-2-yl)-1*H*-benzo[*d*]imidazole (2 mmol; 0.368g) and dimethylformamide (40 ml) were charged in a pressure reactor. The mixture was heated in 140 °C in an oven for 24 hours. After 24 hours the reaction was allowed come down to room temperature. An off-white solid appears in the reaction mixture which was isolated using centrifugation.

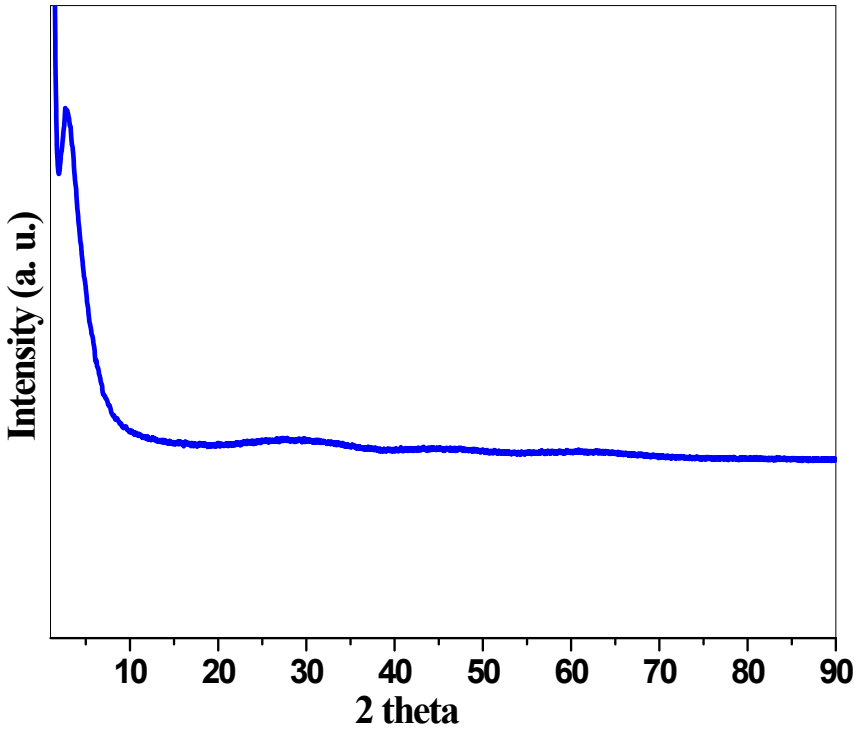
3. Recycling of catalyst:

After the completion of the each reaction, the Ti-ZIF catalyst was recovered using centrifuge, washed with water, dried under vacuum and used for the fresh set of reactants. It was observed that the catalyst remains active even after 3rd cycle and could be reused several times without losing activity.



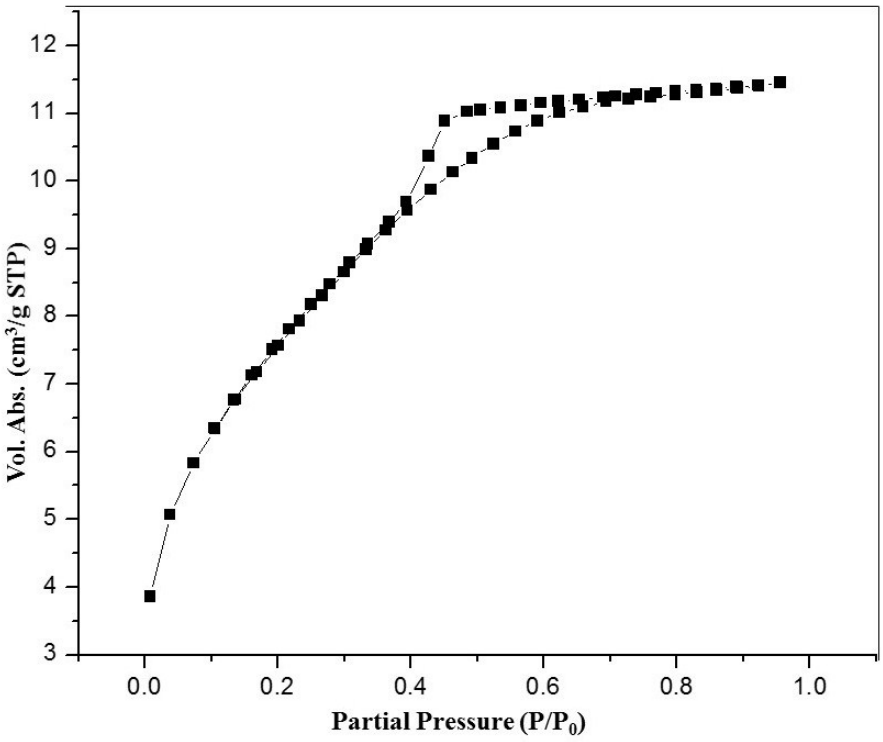
S1. Recycling of Ti-ZIF catalyst

3. XRD spectra of recycled Ti-ZIF catalyst



S2. XRD spectra of recycled Ti-ZIF catalyst

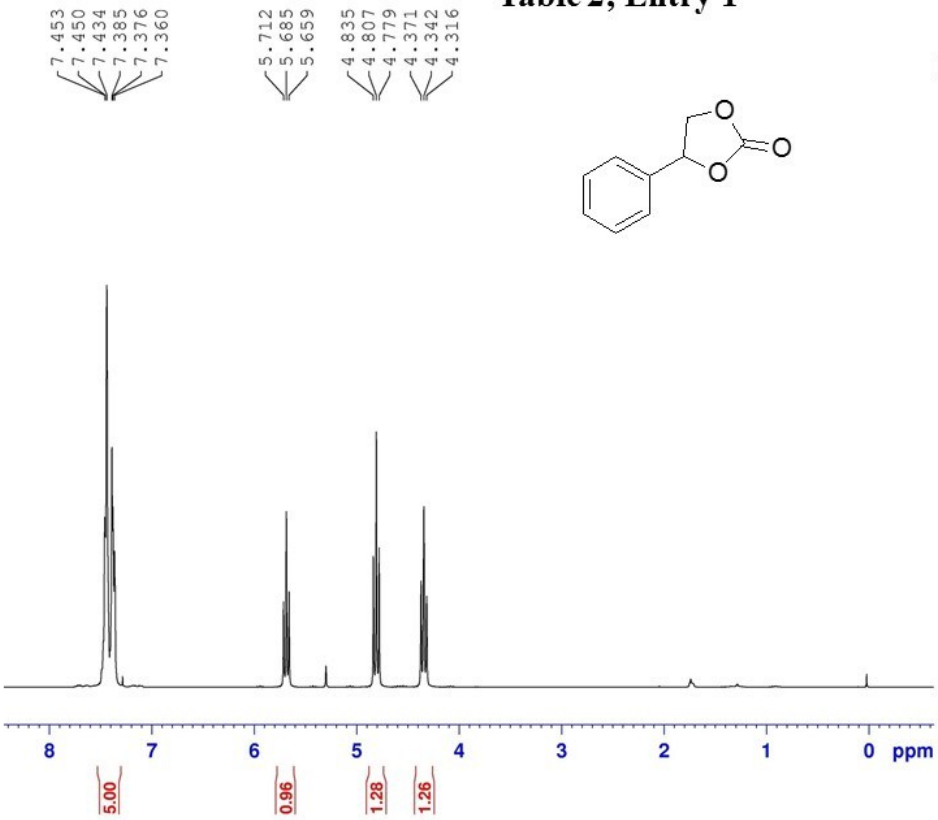
4. N_2 sorption isotherms of recycled Ti-ZIF catalyst



S3. N_2 sorption isotherms of recycled Ti-ZIF catalyst

Table 2; Entry 1

Table 2; Entry 1



```
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PROCNO                   1
Date_             20160205
Time                 15.05
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG                 zg
TD                   32768
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6188.119 Hz
FIDRES            0.188846 Hz
AQ                2.6477852 sec
RG                     181
DW                  80.800 usec
DE                   6.50 usec
TE                  303.0 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   13.00 usec
PL1                   3.20 dB
PL1W         12.02264404 W
SFO1         300.1318534 MHz
SI                   32768
SF           300.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
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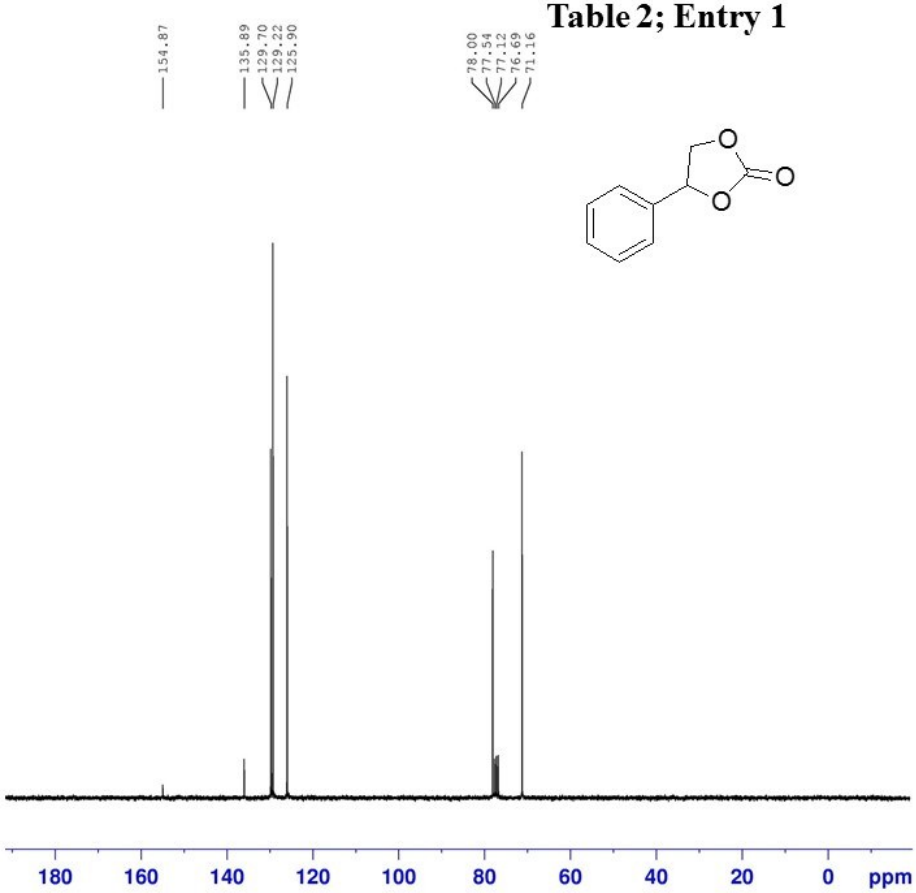
Table 2; Entry 1

Table 2; Entry 1



BRUKER

NAME	NS_STY_CARBONATE
EXPNO	2
PROCNO	1
Date_	20160205
Time	15.48
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgig
TD	32768
SOLVENT	CDC13
NS	500
DS	4
SWH	17985.611 Hz
FIDRES	0.548877 Hz
AQ	0.9110282 sec
RG	8192
DW	27.800 usec
DE	6.50 usec
TE	303.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	1.80 dB
PL1W	49.78760910 W
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	3.20 dB
PL12	18.98 dB
PL2W	12.02264404 W
PL12W	0.31768745 W
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Table 2; Entry 2

Table 2; Entry 2

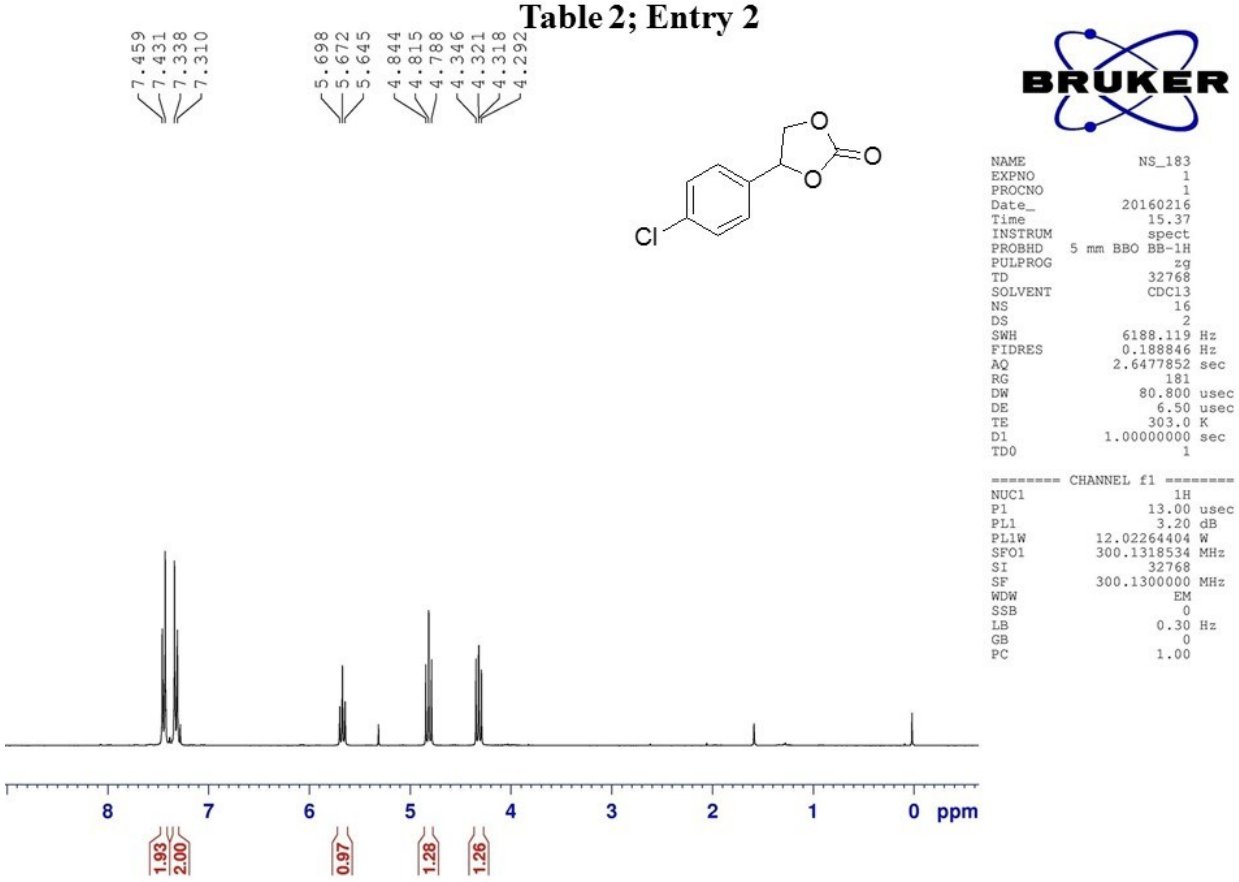
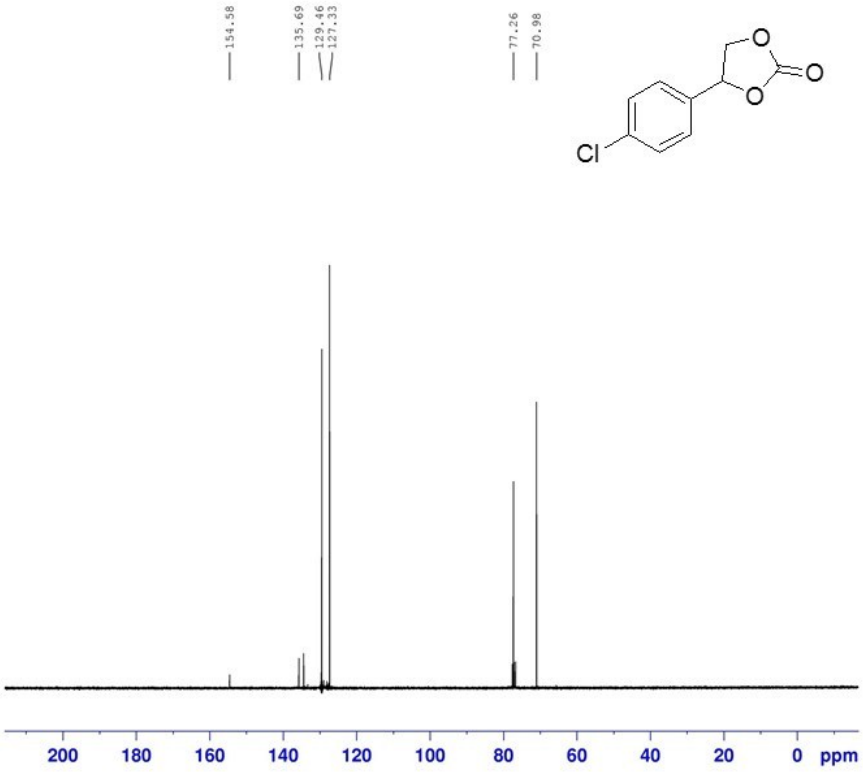


Table 2; Entry 2

Table 2; Entry 2



BRUKER

NAME	NS_183
EXPNO	2
PROCNO	1
Date_	20160216
Time	16.40
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgig
TD	32768
SOLVENT	CDCl3
NS	1024
DS	4
SWH	17985.611 Hz
FIDRES	0.548877 Hz
AQ	0.9110282 sec
RG	8192
DW	27.800 usec
DE	6.50 usec
TE	303.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	1.80 dB
PL1W	49.78760910 W
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	3.20 dB
PL12	18.98 dB
PL2W	12.02264404 W
PL12W	0.31768745 W
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40

Table 2; Entry 3

Table 2; Entry 3

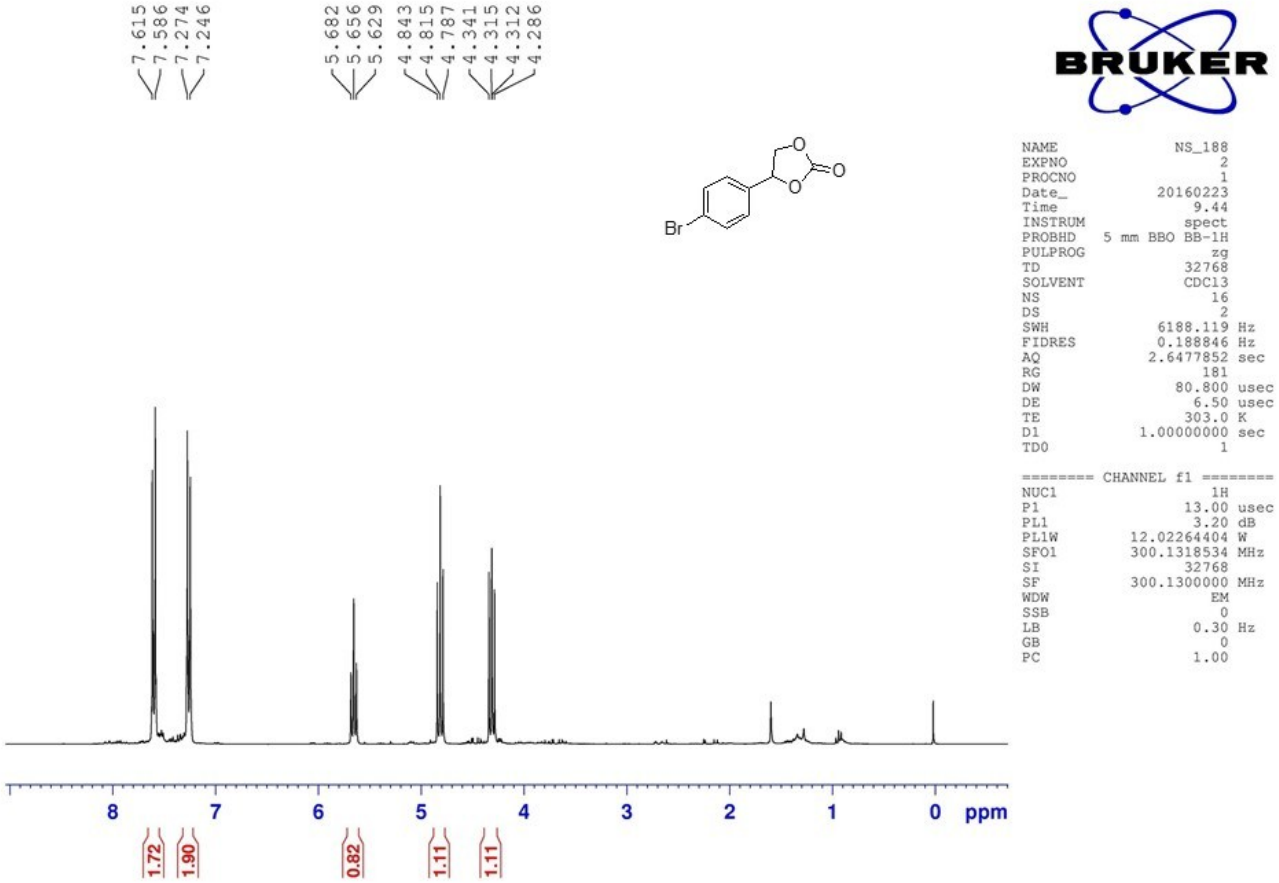


Table 2; Entry 3

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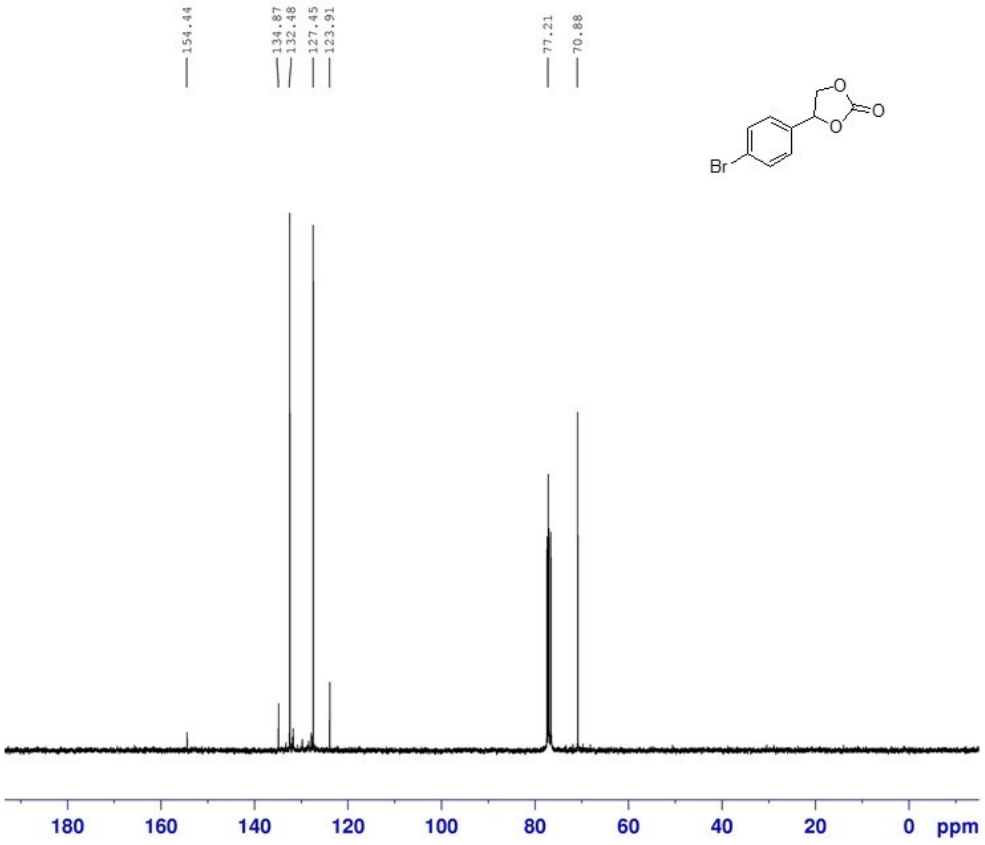
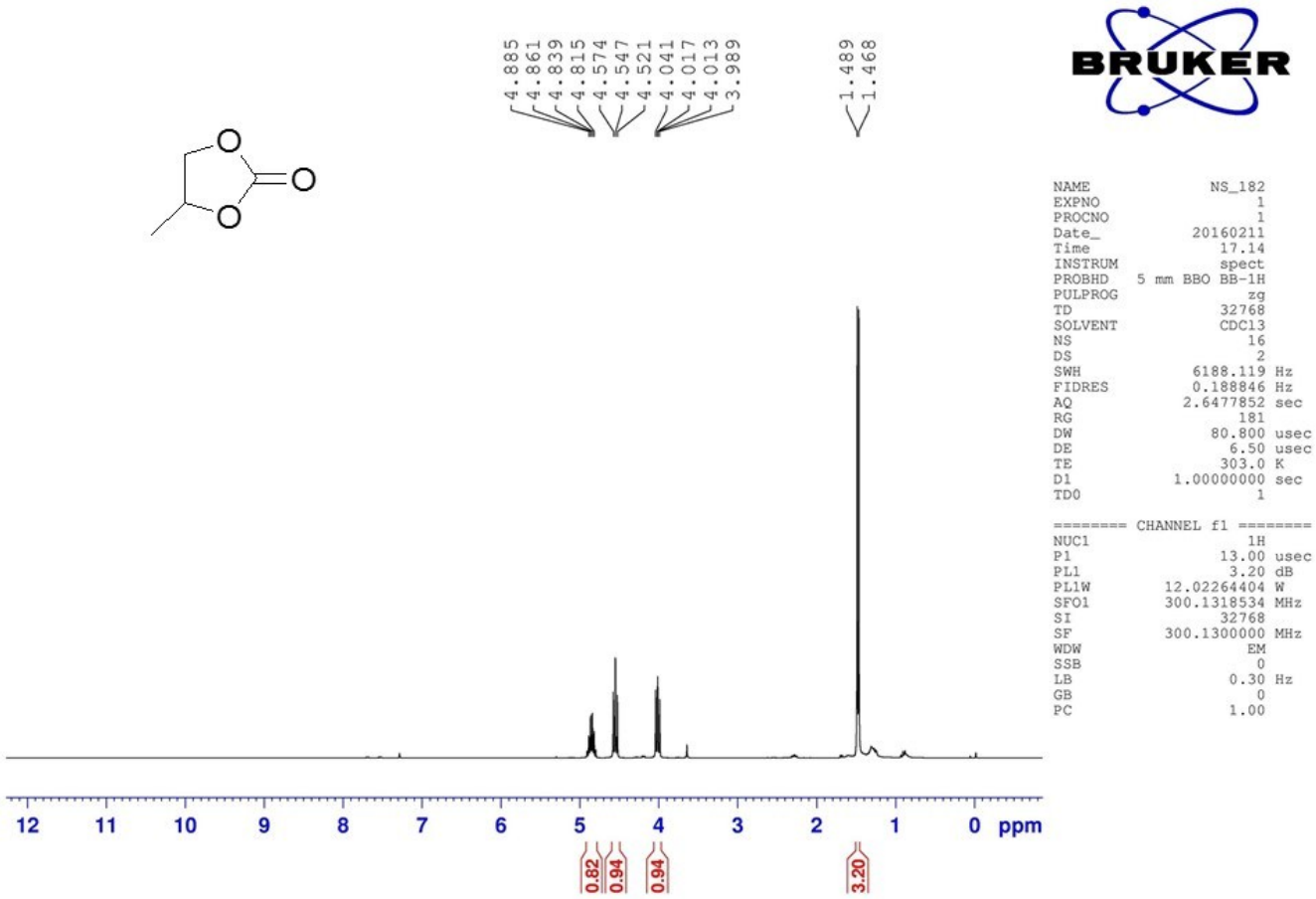


BRUKER

NAME	NS_188
EXPNO	5
PROCNO	1
Date_	20160223
Time	16.22
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgig
TD	32768
SOLVENT	CDCl3
NS	5000
DS	4
SWH	17985.611 Hz
FIDRES	0.548877 Hz
AQ	0.9110282 sec
RG	8192
DW	27.800 usec
DE	6.50 usec
TE	303.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	1.80 dB
PL1W	49.78760910 W
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	3.20 dB
PL12	18.98 dB
PL2W	12.02264404 W
PL12W	0.31768745 W
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Table 2; Entry 4

Table 2; Entry 4



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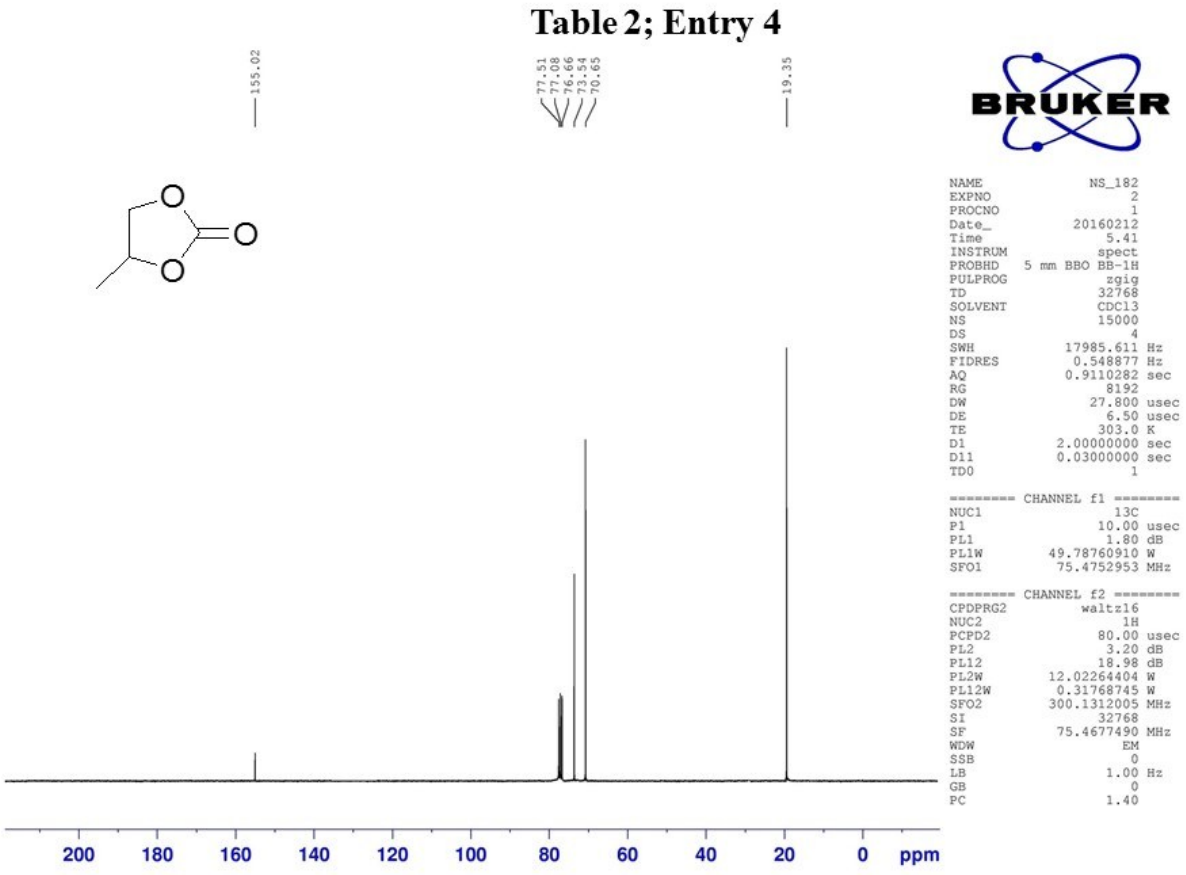

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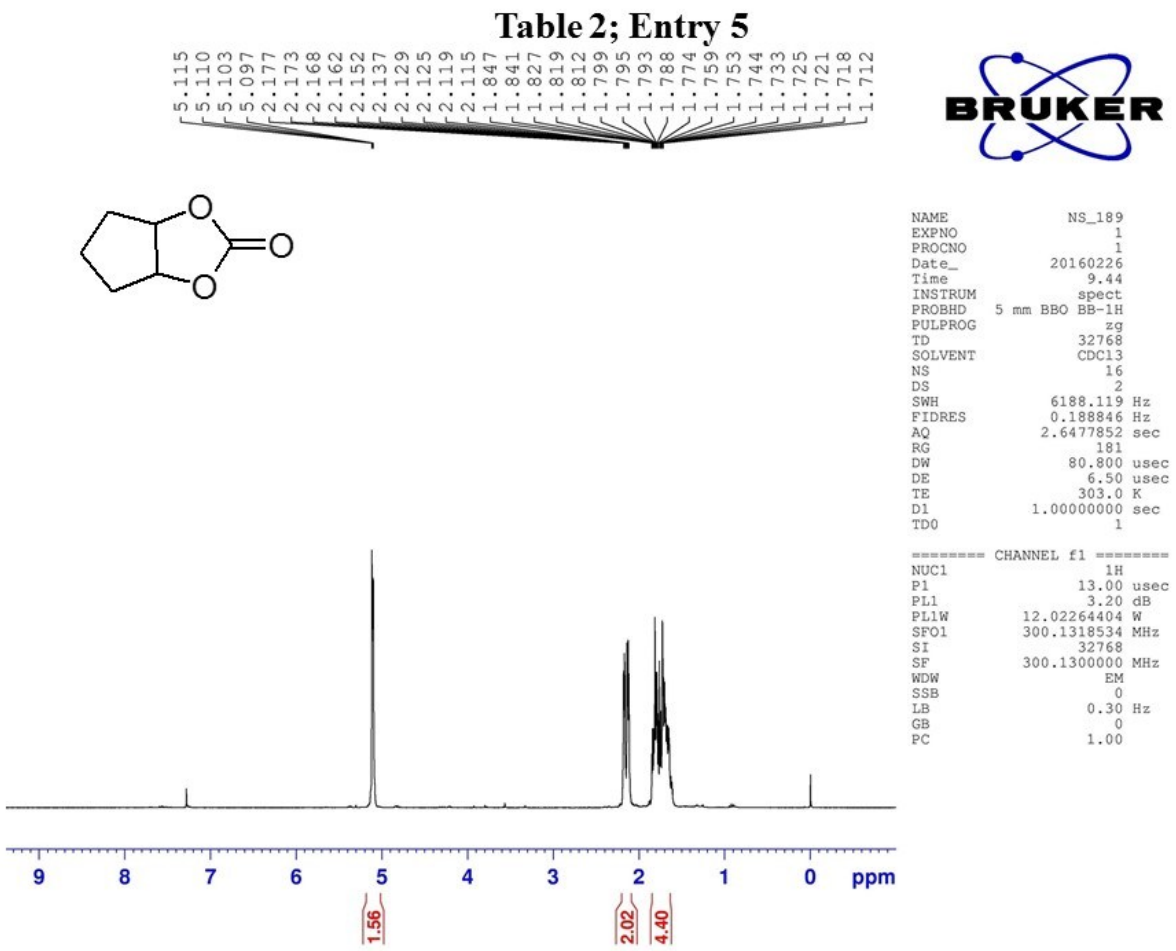
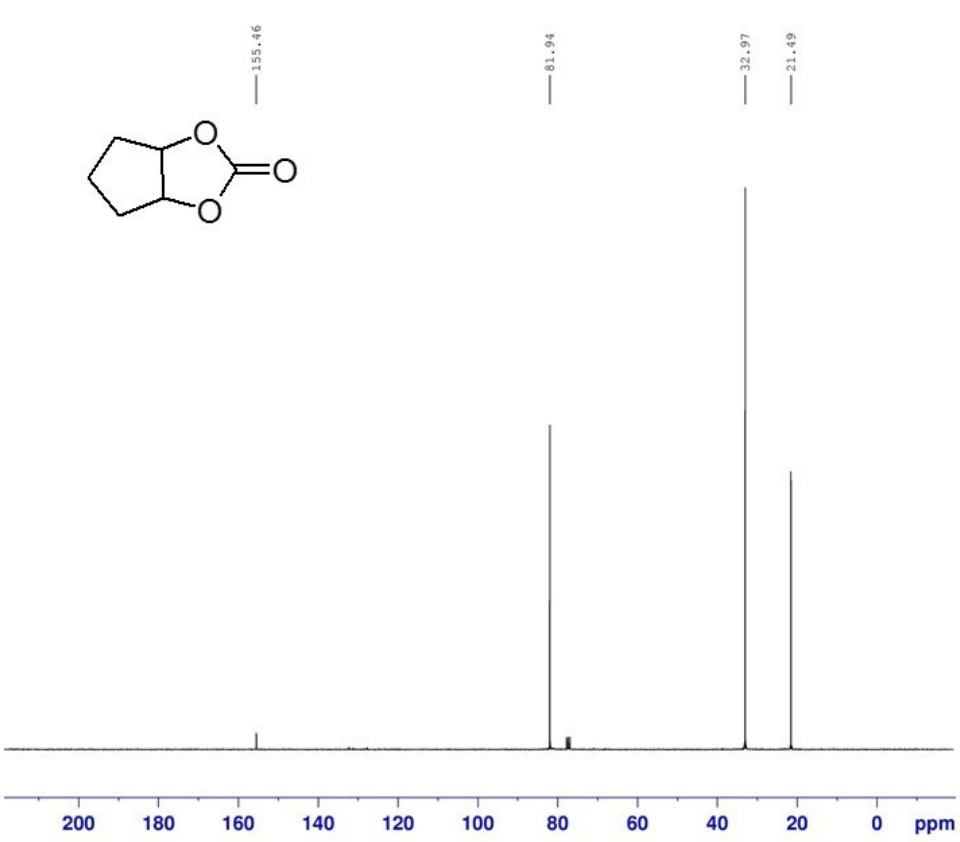


Table 2; Entry 5

Table 2; Entry 5

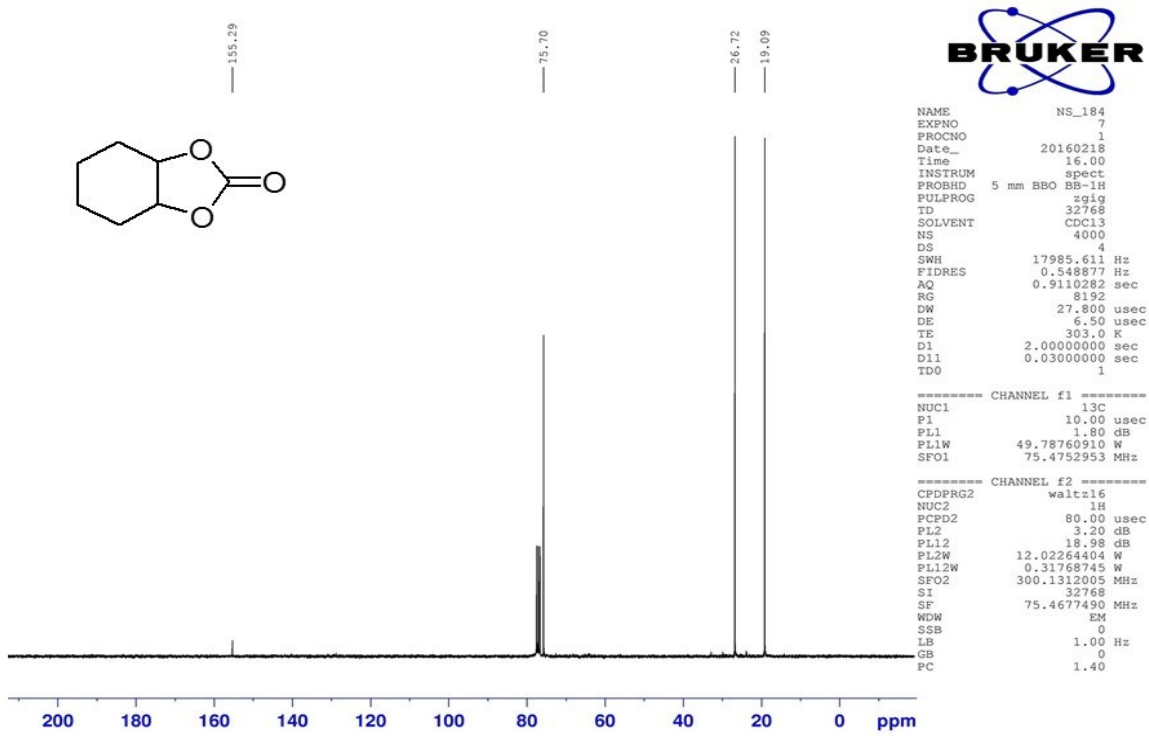


BRUKER

NAME	NS_189
EXPNO	4
PROCNO	1
Date_	20160226
Time	11.54
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgig
TD	32768
SOLVENT	CDCl3
NS	2000
DS	4
SWH	17985.611 Hz
FIDRES	0.548877 Hz
AQ	0.9110282 sec
RG	8192
DW	27.800 usec
DE	6.50 usec
TE	303.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.00 usec
PL1	1.80 dB
PL1W	49.78760910 W
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	3.20 dB
PL12	18.98 dB
PL2W	12.02264404 W
PL12W	0.31768745 W
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Table 2; Entry 6

Table 2; Entry 6

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NAME                NS_184
EXPNO                    7
PROCNO                   1
Date_             20160218
Time                 16.00
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgig
TD                   32768
SOLVENT              CDCl3
NS                    4000
DS                       4
SWH              17985.611 Hz
FIDRES           0.548877 Hz
AQ               0.9110282 sec
RG                    8192
DW                27.800 usec
DE                 6.50 usec
TE                 303.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  10.00 usec
PL1                  1.80 dB
PL1W          49.78760910 W
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                  3.20 dB
PL12                18.98 dB
PL2W          12.02264404 W
PL12W          0.31768745 W
SFO2          300.1312005 MHz
SI                   32768
SF            75.4677490 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```
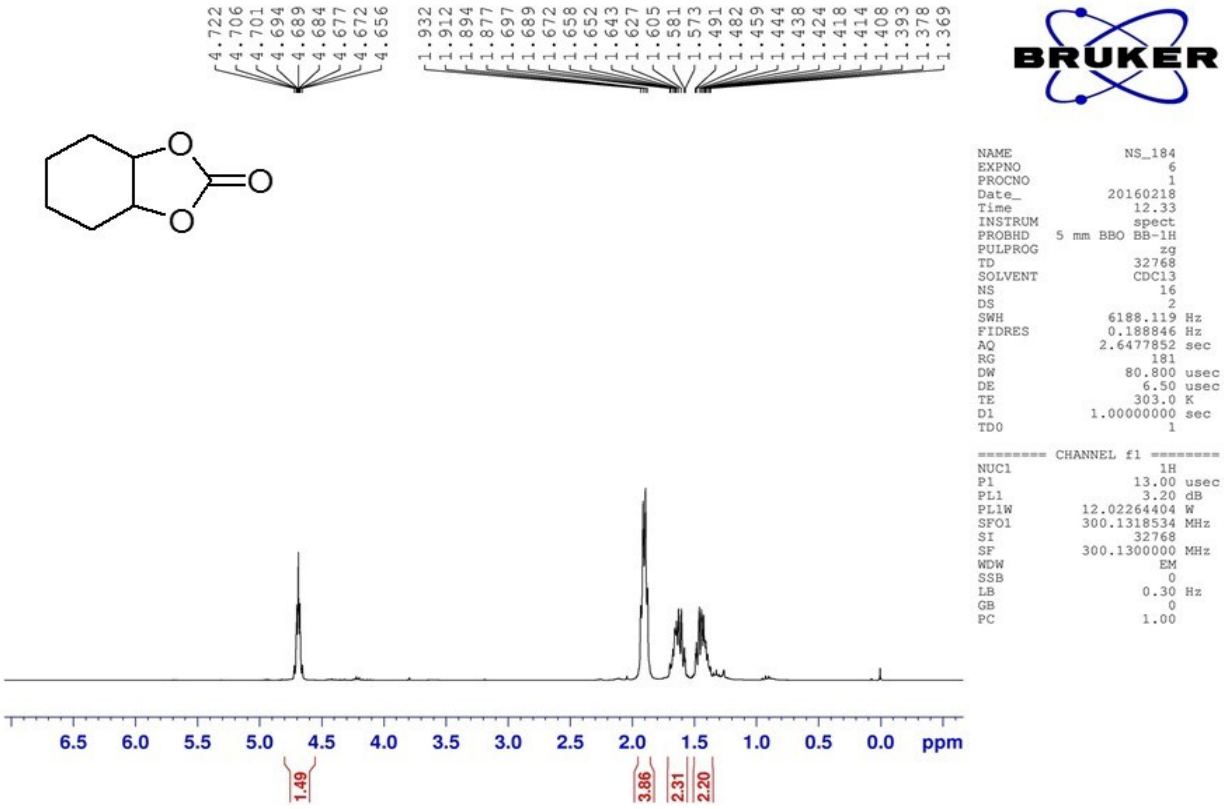

Table 2; Entry 6




```
NAME                NS_184
EXPNO                    6
PROCNO                   1
Date_             20160218
Time                 12.33
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg
TD                   32768
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6188.119 Hz
FIDRES           0.188846 Hz
AQ               2.6477852 sec
RG                     181
DW                80.800 usec
DE                 6.50 usec
TE                 303.0 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   1H
P1                  13.00 usec
PL1                  3.20 dB
PL1W          12.02264404 W
SFO1          300.1318534 MHz
SI                   32768
SF            300.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```