Supporting Information for:

A Simple Catalytic Method for the Regioselective Halogenation of Arenes

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^1H NMR and ^{13}C NMR for compounds **1-Cl** – **14-Cl** Isomer

ms-dk-B-209-fr36-42

Automation directory:

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

Operator: dkalyani

INOVA-500 "Sn.Chem.LSA,UMich.Edu"

Compound 1-Cl Proton

- Relax. delay 0.500 sec
- Pulse 45.0 degrees
- Acq. time 3.000 sec
- Width 7998.4 Hz
- 16 repetitions
- OBSERVE H1, 499.9042537 MHz
- DATA PROCESSING
- Line broadening 0.2 Hz
- FT size 65536
- Total time 1 min. 3 sec

ms-dk-B-218-2-fr40-46

Automation directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Operator: dkalyani

INOVA-400 "Zr.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

2000 repetitions

OBSERVE C13, 100.5712680 MHz

DECOUPLE H1, 399.9669644 MHz

Power 44 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 47 min, 1 sec

Compound 1-Cl Carbon

File: 10-11-11-11-11-11

Acquisition: 10-11-11-11-11-11

Pulse: 10-11-11-11-11-11

Acquisition: 10-11-11-11-11-11

Operator: 10-11-11-11-11-11

File: 10-11-11-11-11-11

INTV: 10-11-11-11-11-11

Relax: delay 0.000 sec

Pulse: 10-11-11-11-11-11

Acq: 10-11-11-11-11-11

Width: 10-11-11-11-11-11

10 repetitions

OBSERVE: 10-11-11-11-11-11

DATA PROCESSING:

Line broadening 0.2 Hz

FF size 65536

total time 1 min. 3 sec

Compound 1-Br Proton

Std Carbon

Automation directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Operator: dkalyani

INOVA-400 "Zr.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

352 repetitions

OBSERVE C13, 100.5712704 MHz

DECOUPLE H1, 399.9669644 MHz

Power 44 dB

continuously on

MALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 23 min, 32 sec

Compound 1-Br Carbon

ms5-dk-8-284

Automation directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Operator: dkalyani

File: ms5-dk-8-284

INQVA-500 "Dy,Chem.LSA.UMich.Edu"

Relax. delay 0.560 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 7998.4 Hz
16 repetitions
OBSERVE H1, 499.9042604 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min. 3 sec

Compound 1-I Proton

S6

mss-dk-8-284-carbon

Automation directory:

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

Operator: dkalyani

INOVA-400 "Zr.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

1000 repetitions

OBSERVE C13, 100.5712788 MHz

DECOUPLE H1, 399.9669644 MHz

Power 44 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 23 min. 32 sec

Compound 1-I Carbon

MS-0K-3-239-11121-125

Pulse Sequence: s2pul

Solvent: Acetone
Ambient temperature
INDVA-400 "Zr"

PULSE SEQUENCE

Pulse 45.0 degrees

Acq. time 2.686 sec

Width 6000.6 Hz

16 repetitions

OBSERVE H1, 399.9670253 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 0 min, 42 sec

Compound 2-Cl Proton

13C OBSERVE

Pulse Sequence: s2pu1

Solvent: Acetone

Ambient temperature

INOVA-400 ¹Zr

PULSE SEQUENCE

Relax. delay 8.800 sec

Pulse 96.6 degrees

Acq. time 1.199 sec

Width 25000.0 Hz

1024 repetitions

OBSERVE C13, 100.5716588 MHz

DECOUPLE H1, 399.9610402 MHz

Power 44 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 35 min, 58 sec

Compound 2-Cl Carbon

Automation directory:

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

Operator: dkalyani

INNOVA-500 "Sn.Chem.LSA.UHich.Edu"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

16 repetitions

OBSERVE H1, 499.9042537 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min. 3 sec

COMPOUND 3-Cl PROTON

mss-dk-9-115-1-2ndcolumn-fr32-42

Automation directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 23.0 C / 296.1 K

Operator: dkalyani

INOVA-400 "Zr.Chem.LSA,UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

320 repetitions

OBSERVE C13, 100.5712659 MHz

DECOUPLE H1, 399.9669644 MHz

Power 38 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 23 min, 32 sec

COMPOUND 3-C1 CARBON

ms: 04-0281-2-n-gmat-fr48-50

Automation directory:

Pulse sequence: zgpg30

Solvent: CDCl₃

Ambient temperature

Operator: dalyam

File: 005-04-0281-2-n-gmat-fr48-50

INQVA-500 "Oy.Chem.LSA,UMich.Eds"

Relax: delay 1.000 sec

Pulse 45.0 degrees

Acq: time 3.000 sec

width 4800.8 Hz

16 repetitions

OBSERVE H1: 300.0732297 MHz

DATA PROCESSING:

Line broadening 0.2 Hz

FT size 32768

Total time 1 min: 4 sec

Compound 4-Cl Proton

Std Carbon

Automation directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Operator: dkalyani

INOVA-400 "Zr.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

320 repetitions

OBSERVE C13, 100.5712734 MHz

DECOUPLE H1, 399.9669644 MHz

Power 44 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 23 min. 32 sec

Compound 4-Cl Carbon

mss-dk-B-274-fr40-50-again

Automation directory:

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

Operator: dkalyani

INOVA-400 "Zr.Chem.LSA.UNich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.500 sec

Width 6399.5 Hz

16 repetitions

OBSERVE H1, 399.9649664 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min, 4 sec

Compound 4-Cl2 Proton

Std Carbon

Compound 4-Cl2 Carbon

Automation directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Operator: dkalyani

INOVA-400 "Zr.Chem.LSA.UMich.Edu"

Relax, delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

416 repetitions

OBSERVE C13, 100.5712752 MHz

DECOUPLE H1, 399.9669644 MHz

Power 44 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 23 min, 32 sec

Automation directory:

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: qanani

Mercury-300 "Zn.Chem.LSA.UMich.Edu"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 4800.8 Hz

16 repetitions

OBSERVE M1, 300.0732420 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 min, 12 sec

Compound 5-Cl Proton

Std Carbon

Automation directory:

Pulse Sequence: s2pu1

Solvent: CDCl₃

Ambient temperature

Operator: dkalyani

INOVA-400 "Zr.Chem.LSA,UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

1000 repetitions

OBSERVE C13: 100.5712676 MHz

DECOUPLE H1: 399.9669644 MHz

Power 44 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 23 min. 32 sec

Compound 5-Cl Carbon

in acetone-d₆

Compound 6-Cl Proton

Automation directory:

Pulse Sequence: s2pu1

Solvent: Acetone

Ambient temperature

Operator: mssanfor

Mercury-300 "Zn.Chem.LSA.UMich.Edu"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 4800.8 Hz

16 repetitions

OBSERVE H1 300.0747909 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 min, 8 sec

S18

13C Carbon

Automation directory:

Pulse Sequence: s2pul

Solvent: Acetone

Ambient temperature

Operator: mssanfor

INDVA-400 "Dr. Chem. LSA, UMich. Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

242 repetitions

OBSERVE C13, 100.5717088 MHz

DECOUPLE H1, 399.9690402 MHz

Power 44 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 39 hr, 8 min, 59 sec

Compound 6-Cl Carbon

Brominated 2-benzoylpyridine for elemental

Automation directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Operator: ardick

INOVA-500 "Sn.Chen.LSA,UMich.Edu"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

16 repetitions

OBSERVE H1, 499.9042609 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min, 3 sec

Compound 7-Br Proton

brominated 2-benzoylpyridine

Automation directory:

Pulse Sequence: s2pu1

Solvent: CDCl₃

Ambient temperature

Operator: ardick

INOVA-400 "Zr.Chem.LSA,UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

3424 repetitions

OBSERVE C13, 100.5712545 MHz

DECOUPLE H1, 399.9669644 MHz

Power 44 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 11 hr, 44 min, 43 sec

Compound 7-Br Carbon

BrCF3Prpy

Automation directory:

Pulse Sequence: s2pu1

Solvent: Acetone

Ambient temperature

Operator: andick

INOWA-500 "Sn.Chem.LSA.UMich.Edu"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

16 repetitions

OBSERVE H1: 499.9066482 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min. 3 sec

Compound 8-Br Proton

CF3PtpyL

Automation directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

File: CF3PtpyL

INQVA-500 "Md.Chem.LSA,UMich.Edu"

Relax. delay 1.000 sec

Pulse 40.0 degrees

Acq. time 1.705 sec

Width 18761.7 Hz

1024 repetitions

OBSERVE C13: 75.4534737 MHz

DECOUPLE H1: 300.0746975 MHz

Power 41 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 46 min. 19 sec

Compound 8-Br Carbon

mg5-dk-b-261-2-repeat-TN46-50

Automation directory:

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

Operator: dkalyani

INOVA-500 "Sn.Chem.LSA,UMich.Edu"

* Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

16 repetitions

OBSERVE H1, 499.9042616 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min. 3 sec

Compound 9-Br Proton

S24

MS-QK-B-300-TF41-55-carbon

Automation directory:

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

Operator: dkalyani

INOVA-400 "Zr.Chem.LSA.Umich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

544 repetitions

OBSERVE C13, 100.5712770 MHz

DECOUPLE H1, 399.9669644 MHz

Power 44 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 23 min, 32 sec

Compound 9-Br Carbon

Compound 10-I Proton

Automation directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Operator: dkalyani

Mercury-300 "Zn.Chem.LSA.UMich.Edu"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 4800.8 Hz

16 repetitions

OBSERVE H1, 300.0732299 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 min, 8 sec

ms5-dk-B-183-33-40-carbon

Automation directory:

Pulse Sequence: s2pu1

Solvent: CDCl₃

Ambient temperature:

Operator: dkalyani

INQVA-500 "Sn, Chem, LSA, UMich, Edu"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30165.9 Hz
1000 repetitions
OBSERVE C13, 125.7010295 MHz
DECOUPLE H1, 499.9072532 MHz
Power 31 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 23 min. 29 sec

Compound 10-I Carbon

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

Operator: dkalyani

INOVA-500 "Sr.Chem.LSA,UMich.Edu"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 7998.4 Hz

16 repetitions

OBSERVE H1 499.9042603 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FI size 65536

Total time 1 min. 3 sec

Compound 11-I Proton

mss-dk-8-231-2ndcol-fr88-104

Automation directory:

Pulse Sequence: s2pu1

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

Operator: dkalyani

INOVA-400 "Zr.Chem.LSA,UMich,EdU"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

1000 repetitions

OBSERVE C13, 100.5712676 MHz

DECOUPLE H1, 399.9669644 MHz

Power 44 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 23 min, 32 sec

Compound 11-I Carbon

ms-dk-8-248-repurified-again

Compound 12-I Proton

Automation directory:

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

Operator: dkalyani

INOVA-400 "Zr.Chem.LSA.UNich.Edu"

Relax_o delay 0.100 sec

Pulse 45.0 degrees

Acq. time 3.500 sec

Width 6399.5 Hz

16 repetitions

OBSERVE H1, 399.9649496 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min, 4 sec

msl-dk-B-248-repurified-carbon

Compound 12-I Carbon

Automation directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Operator: dkalyani

INQVA-400 "Zr.Chem.LSA,UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

1216 repetitions

OBSERVE C13, 100.5712686 MHz

DECOUPLE H1, 399.9669644 MHz

Power 44 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 47 min. 1 sec

ms-metaMechlorination

Automation directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

Operator: dkalyani

Mercury-300 "Zn.Chem.LSA.UMich.Edu"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 4800.8 Hz

16 repetitions

OBSERVE H1, 300.0732301 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 min. 8 sec

Compound 13-Cl Proton

+ 10% REGIOISOMER

Compound 13-Cl Carbon

+ 10% REGIOISOMER.

Acquisition Parameters
 Sample Name: 13-Cl
 Solvent: CDCl3
 Acquisition Date: 10/10/2000
 Acquisition Time: 10:00:00
 Date: 10/10/2000
 Time: 10:00:00
 File Name: 13-Cl
 File Path: 13-Cl
 File Size: 1000000
 File Type: 13-Cl
 File Format: 13-Cl
 File Version: 13-Cl
 File Author: 13-Cl
 File Copyright: 13-Cl
 File License: 13-Cl
 File Contact: 13-Cl
 File Description: 13-Cl
 File Keywords: 13-Cl
 File Comments: 13-Cl
 File Tags: 13-Cl
 File Metadata: 13-Cl
 File History: 13-Cl
 File Status: 13-Cl
 File Version: 13-Cl
 File Author: 13-Cl
 File Copyright: 13-Cl
 File License: 13-Cl
 File Contact: 13-Cl
 File Description: 13-Cl
 File Keywords: 13-Cl
 File Comments: 13-Cl
 File Tags: 13-Cl
 File Metadata: 13-Cl
 File History: 13-Cl
 File Status: 13-Cl

Compound 14-Cl Proton

Automation directory:

Pulse Sequence: s2pu1

Solvent: Acetone

Ambient temperature

Operator: mssanfor

Mercury-300 "Zn.Chem.LSA.UMich.Edu"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 4800.8 Hz

16 repetitions

OBSERVE H1, 300.0747909 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 min, 8 sec

Std Carbon

Compound 14-Cl Carbon

Automation directory:

Pulse Sequence: s2pu1

Solvent: Acetone

Ambient temperature

Operator: mesanfor

INOVA-400 "Zr.Chem.LSA.UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

84 repetitions

OBSERVE C13, 100.5717073 MHz

DECOUPLE H1, 399.9690402 MHz

Power 44 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 091 hr, 29 min, 26 sec

Compound 14-Cl Isomer Proton

Automation directory:

Pulse Sequence: s2pul

Solvent: Acetone

Ambient temperature

Operator: mssanfor

Mercury-300 "Zn.Chem.LSA.UMich.Edu"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 4800.8 Hz

16 repetitions

OBSERVE H1, 300.0747909 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 min. 8 sec

31d Carbon

Automation directory:

Pulse Sequence: s2pul

Solvent: Acetone

Ambient temperature

Operator: mssanfor

INNOVA-400 "Zr.Chem.LSA:UMich.Edu"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24140.0 Hz

124 repetitions

OBSERVE C13, 100.5717073 MHz

DECOUPLE H1, 399.9690402 MHz

Power 44 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 39 hr, 8 min, 59 sec

Compound 14-Cl Isomer Carbon