## Thesis Title

Your name

A thesis submitted to the Faculty of Science,
University of the Witwatersrand,
Johannesburg,
in fulfillment of the requirements for the degree of  $Doctor\ of\ Philosophy$ 

Supervisor: Supervisor name

Johannesburg, November 2016

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#### UNIVERSITY OF THE WITWATERSRAND

## Abstract

Faculty of Science School of Chemistry

Doctor of Philosophy

Thesis Title

by Your name

The Thesis Abstract is written here (and usually kept to just this page). The page is kept centered vertically so can expand into the blank space above the title too...

## Acknowledgements

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## Abbreviations

COSY correlation spectroscopy

CSD Cambridge structure database?  $\underline{\mathbf{A}}$  $\overline{\mathbf{D}}$  $\mathbf{\mathring{A}}$  angstrom  $\mathbf{Ac}$  acetyl  $\mathbf{DCM}$  di-chloromethane  $\mathbf{Ar}$  aryl **DDQ** 2,3-dichloro-5,6-dicyano-1,4-benzoquinone Arom. aromatic **DIA** diisopropylamine **DMAP** 4-N,N-dimethylaminopyridine  $\mathbf{B}$ **DMSO** dimethylsulfoxide  $\mathbf{Bn}$  benzyl  $\mathbf{E}$ Boc tert-butyl carbonate EIMS electron ionisation mass spec-**BP** boiling point troscopy BuLi butyl lithium ESIMS electrospray ionisation mass spectroscopy  $\mathbf{C}$  $\mathbf{Et}$  ethyl  $^{\circ}\mathbf{C}$  degrees Celsius EtOAc ethyl acetate CIMS Ceric ammonium nitrate eq equivalents CIMS chemical ionisation mass spec-Η troscopy

h hour

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HMBC heteronuclear multiple bond correlation	PMB para-methoxy-benzyl
HSQC heteronuclear single-quantum correlation	<u>R</u>
	rt room temperature
Ī	
<i>i</i> -Pr <i>iso</i> -propyl	${f T}$
IR infrared	${\bf TBAF} \ \ {\bf tetra-butyl-ammonium-fluoride}$
${f \underline{M}}$	TBDMS tert-butyldimethylsilyl
	<i>t</i> -Bu <i>tert</i> -butyl
Me methyl	TEA triethylamine
min minute	Tetrakis $Pd(PPh_3)_3)$
MP melting point	THF tetrahydrofuran
${f N}$	TLC thin layer chromatography
NBS N-bromo-succinimide	$\mathbf{TMS} \ \ \mathbf{tetramethyl\text{-}silane/trimethyl\text{-}}$
<i>n</i> -Bu <i>n</i> -butyl	silane
NMP N-methyl pyrilidone	Tosyl toluenesulfonyl
NMR nuclear magnetic resonance	<b>TOF</b> Turn over frequency
n-Pr $n$ -propyl	TON Turn over number
<u>P</u>	${f Q}$
Ph phenyl	quant quantitative

## Chapter 1

## Example

### 1.1 Sectional example

Now I will reference Scheme 1.1 in text.

$$\begin{array}{c|c} & & & \\ \hline \\ N \\ N \\ 1 \\ \end{array} \begin{array}{c} & \\ \hline \\ BnBr \\ \hline \\ KOH \\ \end{array} \begin{array}{c} & \\ \hline \\ N \\ \hline \\ \end{array} \begin{array}{c} & \\ \hline \\ N \\ \hline \\ \end{array} \begin{array}{c} & \\ \hline \\ NaOH \\ \end{array} \begin{array}{c} & \\$$

Scheme 1.1: The synthesis of **3** from the indole by formylation and benzyl protection.

 $\mathrm{CH_{3}(C=O)CH_{3}}$  or  $\mathrm{MgSO_{4}}$ 

# Chapter 2

## Introduction

## Chapter 3

# Experimental templates and examples

#### 3.1 NMR

```
NH2 - (s, 2H, N\underline{\mathbf{H}}_2)

NH - (s, 1H, N\underline{\mathbf{H}})

CH3 - H - (s, 3H, C\underline{\mathbf{H}}_3) C - (\underline{\mathbf{C}}H_3)

Si(CH3)3 - C - (\mathrm{Si}(\underline{\mathbf{C}}H_3)_3)

C(CH3)3 (tert-carbon underlined) - C - (\underline{\mathbf{C}}(\mathrm{CH}_3)_3)

C(CH3)3 (methyl underlined) - C - (\mathrm{C}(\underline{\mathbf{C}}H_3)_3)

C CH - H - (s, 1H, \equiv \underline{\mathbf{C}}\underline{\mathbf{H}}) C - (\equiv \underline{\mathbf{C}}H)

C-C C - C - (\underline{\mathbf{C}}-\underline{\mathbf{C}}\equiv\mathbf{C})

N-C=O - C - (N-\underline{\mathbf{C}}=\mathbf{O})

aromatic C - (C-\mathrm{arom.})

CH2 - H - C\underline{\mathbf{H}}_2 C - \underline{\mathbf{C}}H<sub>2</sub>
```

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#### 3.2 experimental entrty

#### Phenol (4)

Yield:

MP:

IR (cm<sup>-1</sup>):  $\bar{v}$ 

<sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>):  $\delta$ 

 $^{13}$ C NMR (75MHz, CDCl<sub>3</sub>):  $\delta$ 

HRMS:

()

Yield:

MP:

IR (cm<sup>-1</sup>):  $\bar{v}$ 

<sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>):  $\delta$ 

 $^{13}$ C NMR (75MHz, CDCl<sub>3</sub>):  $\delta$ 

HRMS:

#### 3.3 crystal tables

#### 3.4 chemfig

Boc ([:30]-([2]=O)([:330]-O([:30]-([2]-)([:30]-)([:330]-)

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Table 3.1: Crystal data of

Empirical formula	$C_{11}H_{14}N_2Si_1$
Formula weight	
Temperature	K
Wavelength	Å
Crystal system	
Space group	$\mathbf{C}$
Unit cell dimensions	
a = A	$lpha={}^{\circ}$
b = A	$eta$ = $^{\circ}$
c = Å	$egin{array}{l} lpha = ^{\circ} \ eta = ^{\circ} \ \gamma = ^{\circ} \end{array}$
Volume	$\rm \AA^3$
Z	
Density (calculated)	$Mg/m^3$
Absorption coefficient	$\mathrm{mm}^{-1}$
F(000)	
Crystal size	$\mathrm{mm}^3$

Table 3.2: Data collection of

$\theta$ range for data collection	$^{\circ}$ to $^{\circ}$
Index ranges	$- \preceq h \preceq, - \preceq k \preceq, - \preceq l \preceq$
Reflections collected	
Independent reflections	[R(int) = ]
Completeness to $\theta = {}^{\circ}$	%

Table 3.3: Refinement of

Refinement method	Full-matrix least-squares on $F^2$	
Data / restraints / parameters	/ /	
Goodness-of-fit on $F^2$		
Final R indices $[I > 2\sigma(I)]$	R1 = , wR2 =	
R indices (all data)	R1 = , wR2 =	
Largest diff. peak and hole	and - $e.Å^{-3}$	

# Appendix A