



UNIVERSITI PUTRA MALAYSIA

**MESOGENIC PROPERTIES OF A SERIES OF SYNTHESIZED
CALAMITIC LIQUID CRYSTALS CONTAINING 1,2,4,5-TETRAZINE
MOIETIES**

NOOR HAFIZAH ABDUL HALIM

FS 2009 28



**MESOGENIC PROPERTIES OF A SERIES OF
SYNTHESIZED CALAMITIC LIQUID CRYSTALS
CONTAINING 1,2,4,5-TETRAZINE MOIETIES**

NOOR HAFIZAH ABDUL HALIM

**MASTER OF SCIENCE
UNIVERSITI PUTRA MALAYSIA**

2009



**MESOGENIC PROPERTIES OF A SERIES OF SYNTHESIZED CALAMITIC
LIQUID CRYSTALS CONTAINING 1,2,4,5-TETRAZINE MOIETIES**

NOOR HAFIZAH ABDUL HALIM

**MASTER OF SCIENCE
UNIVERSITI PUTRA MALAYSIA**

2009



**MESOGENIC PROPERTIES OF A SERIES OF SYNTHESIZED CALAMITIC
LIQUID CRYSTALS CONTAINING 1,2,4,5-TETRAZINE MOIETIES**

By

NOOR HAFIZAH ABDUL HALIM

**Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in
Fulfilment of the Requirements for the Degree of Master of Science**

June 2009



Abstract of thesis presented to the senate of Universiti Putra Malaysia in fulfilment of requirement for the degree of Master of Science

MESOGENIC PROPERTIES OF A SERIES OF SYNTHESIZED CALAMITIC LIQUID CRYSTALS CONTAINING 1,2,4,5-TETRAZINE MOIETIES

By

NOOR HAFIZAH ABDUL HALIM

June 2009

Chairman : Associate Professor Dr. Sidik Silong

Faculty : Science

In this research, a series of calamitic liquid crystal containing 1,2,4,5-tetrazine moieties have been synthesized. 1,2,4,5-tetrazine is a mesomorphic compound containing heterocyclic units and such structures have greater possibilities to obtain mesogenic molecules. All compounds were synthesized by esterification of $\text{HOC}_6\text{H}_4\text{C}_2\text{N}_4\text{C}_6\text{H}_4\text{OH}$ with carboxylic acids that vary in substituents chain lengths. The structures of the liquid crystal compounds were elucidated based on FT-IR, mass spectroscopy, CHN and NMR analyses. The infrared spectra of the compounds showed the characteristic of the tetrazine and ester functional group for $\nu\text{C}=\text{O}$, $\nu\text{C}=\text{C}$, $\nu\text{C}=\text{N}$, $\nu\text{N}-\text{N}$ and $\nu\text{C}-\text{O}$ at ($1750-1758\text{ cm}^{-1}$), ($1602-1604\text{ cm}^{-1}$), ($1318-1396\text{ cm}^{-1}$), ($1142-1168\text{ cm}^{-1}$) and ($1016-1102\text{ cm}^{-1}$). The elemental analyses agree with the expected formula $\text{R}-\text{C}_6\text{H}_4\text{C}_2\text{N}_4\text{C}_6\text{H}_4-\text{R}$ where $\text{R} = \text{C}_2\text{H}_5$ (FZ-4), C_4H_9 (Isobutyl) (FZ-49E), C_5H_{11} (FZ-37B), $\text{C}_{11}\text{H}_{23}$ (FZ-53), $\text{C}_{15}\text{H}_{31}$ (FZ-34A) and $\text{C}_{17}\text{H}_{35}$ (FZ-35A). The ^1H NMR spectra reflected the high symmetry of the molecules



with the benzene protons appeared as a doublet at $\delta(8.69-8.67\text{ppm})$ and $\delta(7.36-7.34\text{ppm})$, respectively. The ^{13}C signals for the 1,2,4,5-tetrazine, C=O and C-O appeared at $\delta(163.30-163.25)$, $\delta(171.82-171.02\text{ppm})$ and $\delta(154.48-154.40\text{ppm})$, respectively. Differential scanning calorimetry (DSC) and polarizing optical microscopy (POM) analyses of FZ-37B, FZ-53, FZ-34A and FZ-35A revealed the existence of smectic and schlieren smectic mesophases.



Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk Ijazah Master Sains

**SIFAT-SIFAT MESOGENIK SATU SIRI CECAIR HABLUR KALAMITIK
TERSINTESIS MENGANDUNGI BAHAGIAN 1,2,4,5-TETRAZINE**

Oleh

NOOR HAFIZAH ABDUL HALIM

Jun 2009

Pengerusi : Profesor Madya Dr. Sidik Silong

Fakulti : Sains

Dalam kajian ini, satu siri cecair hablur kalamitik mengandungi bahagian 1,2,4,5-tetrazine telah disintesis. 1,2,4,5-tetrazine adalah satu sebatian mesomorfik yang mengandungi unit-unit heterosiklik dan struktur seperti itu berkemungkinan besar untuk membentuk molekul mesogenik. Semua sebatian telah disintesis melalui pengesteran $\text{HO-C}_6\text{H}_4\text{-C}_2\text{N}_4\text{-C}_6\text{H}_4\text{-OH}$ dengan asid karboksilik yang berbeza dalam penukarganti rantai panjang. Struktur sebatian cecair hablur ini dijelaskan berasaskan kepada FT-IR, spektroskopi jisim (MS) dan analisis CHN serta NMR. Spektrum infra-merah bagi sebatian menunjukkan ciri-ciri kumpulan berfungsi tetrazin dan ester bagi $\nu\text{C}=\text{O}$, $\nu\text{C}=\text{C}$, $\nu\text{C}=\text{N}$, $\nu\text{N}-\text{N}$ dan $\nu\text{C}-\text{O}$ pada ($1750\text{-}1758\text{ cm}^{-1}$), ($1602\text{-}1604\text{ cm}^{-1}$), ($1318\text{-}1396\text{ cm}^{-1}$), ($1142\text{-}1168\text{ cm}^{-1}$) dan ($1016\text{-}1102\text{ cm}^{-1}$). Analisis unsur bersetuju dengan formula yang dicadangkan $\text{R-C}_6\text{H}_4\text{-C}_2\text{N}_4\text{-C}_6\text{H}_4\text{-R}$ di mana $\text{R} = \text{C}_2\text{H}_5$ (FZ-4), C_4H_9 (Isobutyl) (FZ-49E), C_5H_{11} (FZ-37B), $\text{C}_{11}\text{H}_{23}$ (FZ-53), $\text{C}_{15}\text{H}_{31}$ (FZ-34A) and $\text{C}_{17}\text{H}_{35}$ (FZ-35A). Spektrum ^1H



NMR menggambarkan ketinggian simetri sebatian dengan proton-proton benzena muncul sebagai dublet pada $\delta(8.69-8.67\text{ppm})$ dan $\delta(7.36-7.34\text{ppm})$. Puncak ^{13}C bagi 1,2,4,5-tetrazine, C=O dan C-O muncul di $\delta(163.30-163.25)$, $\delta(171.82-171.02\text{ppm})$ dan $\delta(154.48-154.40\text{ppm})$. Analisis teknik kalorimeter imbasan keberdaan (DSC) dan mikroskopi berkutub optik (OPM) bagi FZ-37B, FZ-53, FZ-34A dan FZ-35A mendedahkan kehadiran mesofasa-mesofasa smektik dan smektik yang memancar.

ACKNOWLEDGEMENT

Thankfully to God for giving me strength, patience and confidence in finishing my research project also this thesis. I wish to embrace my acknowledgements to all those people who enormously help and support me during my entire MSc programme.

First of all, I would like to express my deepest and warmest sense of thanks to my project supervisor Associate Professor Dr. Sidik Silong and my Co-Supervisor Dr. Mohammad Zaki Abdul Rahman for welcoming me to their liquid crystal research group and for their invaluable advice, guidance, comments and also criticism during my master research project.

Thanks are also to all the technical staffs of the Chemistry Department in particular, for their assistance and cooperation towards the success of this project. I would like to extend my gratitude to Mr. Abdul Salam and Miss Sheila for invaluable discussions relating to this project.

Sincere thanks to my lovely parents and my siblings for their care and support, who contributed towards the success of this project. Thanks also for my entire friend for their constant support and most importantly their laughs.

Finally, I would like to thank The University of Putra Malaysia and IRPA Grant (06-01-04-SSF0144) for the facilities and financial support.



I certify that a Thesis Examination Committee has met on 23 June 2009 to conduct the final examination of Noor Hafizah binti Abdul Halim on her thesis entitled “Mesogenic Properties of a Series of Synthesized Calamitic Liquid Crystals Containing 1,2,4,5-Tetrazine Moieties” in accordance with the Universities and University Colleges Act 1971 and the Constitution of the Universiti putra Malaysia [P.U.(A) 106] 15 March 1998. The committee recommends that the student be awarded the Master of Science.

Members of the Thesis Examination Committee were as follows:

Md. Jelas Haron, PhD

Professor
Faculty of Science
Universiti Putra Malaysia
(Chairman)

Anuar Kassim, PhD

Professor
Faculty of Science
Universiti Putra Malaysia
(Internal Examiner)

Mawardi Rahmani, PhD

Professor
Faculty of Science
Universiti Putra Malaysia
(Internal Examiner)

Mohammad Kassim, PhD

Associate Professor
Faculty of Science and Technology
Universiti Kebangsaan Malaysia
(External Examiner)

BUJANG KIM HUAT, PhD

Professor and Deputy Dean
School of Graduate Studies
Universiti Putra Malaysia

Date : 15 October 2009



This thesis was submitted to the Senate of Universiti Putra Malaysia has been accepted as fulfilment of the requirement for the degree of Master of Science. The members of the Supervisory Committee were as follows:

Sidik Silong, PhD

Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Chairman)

Mohammad Zaki Abdul Rahman, PhD

Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Member)

HASANAH MOHD GHAZALI, PhD

Professor and Dean
School of Graduate Studies
Universiti Putra Malaysia

Date : 16 November 2009



DECLARATION

I hereby declare that the thesis is based on my original work except for quotations and citations, which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at UPM or other institutions.

NOOR HAFIZAH ABDUL HALIM

Date : 4 January 2010



TABLE OF CONTENTS

	Page
ABSTRACT	ii
ABSTRAK	iv
ACKNOWLEDGEMENTS	vi
APPROVAL	vii
DECLARATION	ix
LIST OF TABLES	xiii
LIST OF SCHEMES	xiv
LIST OF FIGURES	xv
LIST OF ABBREVIATIONS	xxi
CHAPTER	
1 INTRODUCTION	1
1.1 A Brief History of Liquid Crystals	1
1.2 Introduction to Liquid Crystals	2
1.3 Types of Liquid Crystals (LCs)	3
1.4 Calamitic LCs	4
1.5 Molecular Geometry of Molecules Which Form Thermotropic Calamitic Liquid Crystals	5
1.6 Calamitic LCs Phases	6
1.6.1 Nematic Phases	6
1.6.2 Smectic Phases	7
1.6.3 Rule of the Phase Sequences	7
1.7 Calamitic LC Textures	8
1.7.1 Homeotropic or pseudoisotropic texture	8
1.7.2 The Focal-conic Fan Texture	9
1.7.3 The Polygonal Texture	10
1.7.4 The Schlieren Texture	11
1.7.5 The Mosaic Texture	12
1.8 Calamitic Liquid Crystals containing 1,2,4,5-tetrazine	13
1.9 Objectives	15
2 LITERATURE REVIEW	16
2.1 Substituted 1,2,4,5-Tetrazines and their chain length synthesis	16
2.2 Physical Properties of tetrazine and Its Theoretical Considerations	19
2.3 Rod-core mesogens, chain length substituent effect and phase behavior	20
3 EXPERIMENTAL	23
3.1 Chemicals	23



3.2	Instrumentations	24
3.3	Methodology	27
3.3.1	Preparation of Anhydrous Hydrazine	27
3.3.2	Synthesis of 4-(1,2-dihydro-6-(4-hydroxyphenyl)-1,2,4,5-tetrazin-3-yl)phenol (FZ-1)	28
3.3.3	Synthesis of Characterization of 4-[6-(4-hydroxyphenyl)-1,2,4,5-tetrazine-3-yl]phenol (FZ-2)	28
3.3.4	Synthesis of propionic acid 4-[6-(4-propionoyloxy-phenyl)-1,2,4,5-tetrazin-3-yl]-phenyl ester FZ-4	29
3.3.5	Synthesis of 3-Methyl-butyric acid 4-{6-[4-(3-methyl-butyryloxy)-phenyl]-[1,2,4,5]tetrazin-3-yl}-phenyl ester (FZ-49E)	30
3.3.6	Synthesis of Hexanoic acid 4-[6-(4-hexanoyloxy-phenyl)-1,2,4,5-tetrazine-3yl]-phenyl ester (FZ-37B)	30
3.3.7	Synthesis of Dodecanoic acid 4-[6-(4-dodecanoyloxy-phenyl)-[1,2,4,5]tetrazin-3-yl]-phenyl ester (FZ-53)	31
3.3.8	Synthesis of Hexadecanoic acid 4-[6-(4-hexadecanoyloxy-phenyl)-[1,2,4,5]tetrazin-3-yl]-phenyl ester (FZ-34A)	31
3.3.9	Synthesis of Octadecanoic acid 4-[6-(4-octadecanoyloxy-phenyl)-[1,2,4,5]tetrazin-3-yl]-phenyl ester (FZ-35A)	32
4	RESULTS AND DISCUSSION	33
4.1	Synthesis	33
4.2	Characterization	36
4.2.1	Characterization of 4-(1,2-dihydro-6-(4-hydroxyphenyl)-1,2,4,5-tetrazin-3-yl)phenol (FZ-1)	36
4.2.2	Characterization of 4-[6-(4-hydroxyphenyl)-1,2,4,5-tetrazine-3-yl]phenol (FZ-2)	40
4.2.3	Characterization of propionic acid 4-[6-(4-propionoyloxy-phenyl)-1,2,4,5-tetrazin-3-yl]-phenyl ester (FZ-4)	50
4.2.4	Characterization of 3-Methyl-butyric acid 4-{6-[4-(3-methyl-butyryloxy)-phenyl]-[1,2,4,5]tetrazin-3-yl}-phenyl ester (FZ-49E)	61
4.2.5	Characterization of Hexanoic acid 4-[6-(4-hexanoyloxy-phenyl)-1,2,4,5-tetrazine-3yl]-phenyl ester (FZ-37B)	71
4.2.6	Characterization of Dodecanoic acid 4-[6-(4-dodecanoyloxy-phenyl)-[1,2,4,5]tetrazin-3-yl]-phenyl ester (FZ-53)	82
4.2.7	Characterization of Hexadecanoic acid 4-[6-(4-hexadecanoyloxy-phenyl)-[1,2,4,5]tetrazin-3-yl]-	94



	phenyl ester (FZ-34A)	
4.2.8	Characterization of Octadecanoic acid 4-[6-(4-octadecanoyloxy-phenyl)-[1,2,4,5]tetrazin-3-yl]-phenyl ester (FZ-35A)	105
5	CONCLUSION	119
	REFERENCES	120
	BIODATA OF STUDENT	125



LIST OF TABLES

Table		Page
1	The list of chemicals used in study	24
2	Infrared Data of the compounds	116
3	CHN data analyses and yield of the compounds	117
4	Transition temperature of compounds synthesized	118



LIST OF SCHEMES

Scheme		Page
1	Preparation of tetrazine	17
2	Tetrazole photolysis	17
3	Route of synthesis 3,6-disubstituted-1,2,4,5-tetrazines	18
4	Esterification of alcohol biphenyl substrate with acid to furnish an ester using DCC and DMAP as catalyst.	18
5	Esterification of alcohol with POMBOH to furnish POMB ester using DCC and DMAP as catalyst.	19
6	The influence of nitrogen substituents on the mesogeneity	21
7	Reaction scheme and conditions for the synthesis of rod-like liquid crystal compounds containing 1,2,4,5-tetrazines moieties	33
8	Mechanism of fragmentation for FZ-1	39
9	Mechanism of fragmentation for FZ-2	44
10	Mechanism of fragmentation for FZ-4	54



LIST OF FIGURES

Figure		Page
1	The average alignment of the molecule for each phase	3
2	Cartoon representation of calamitics LCs	5
3	The natural texture of the smectic B phase obtained on cooling the isotropic liquid, the black areas are homeotropic S _B .	9
4	The focal-conic fan texture of the smectic A phase.	10
5	The polygonal texture of the smectic A phase.	11
6	(a) point singularity with four brushes; (b) point singularity with two brushes	12
7	The schlieren texture of the smectic C phase.	12
8	The mosaic texture of the smectic B phase.	13
9	Structure of tetrazine	16
10	Structure of 3-bromo-6-phenyl-1,2,4,5-tetrazine	20
11	Structure of 3,6-bis -(4-aminophenyl)-1,2,4,5-tetrazine	20
12	The apparatus setup for anhydrous hydrazine	27
13	Structures of liquid crystal molecules showing various lengths of alkyl groups.	35
14	IR Spectrum of FZ-1, all the labeled peaks are representing stretching frequency of the appropriate functional groups, except for those mentioned other wise.	37
15	EIMS Spectrum of FZ-1	38



16	IR Spectrum of FZ-2, all the labeled peaks are representing stretching frequency of the appropriate functional groups, except for those mentioned other wise.	42
17	EIMS Spectrum of FZ-2	43
18	¹ H NMR spectrum of FZ-2 (400 MHz, DMSO)(expanded)	45
19	¹³ C NMR spectrum of FZ-2 (400 MHz, DMSO)	46
20	DEPT spectrum of FZ-2 (100 MHz, DMSO)	47
21	DSC Thermogram of FZ-2 on second cooling and second heating	48
22	Solid form of FZ-2	49
23	Isotropic form of FZ-2 at 306°C	49
24	IR Spectrum of FZ-4, all the labeled peaks are representing stretching frequency of the appropriate functional groups, except for those mentioned other wise	52
25	EIMS Spectrum of FZ-4	53
26	¹ H NMR spectrum of FZ-4 (400 MHz, CDCl ₃) (expanded)	55
27	¹³ C NMR spectrum of FZ-4 (400 MHz, CDCl ₃)	56
28	DEPT spectrum of FZ-4 (100 MHz, CDCl ₃)	57
29	DSC Thermogram of FZ-4 on second cooling and second heating	58
30	FZ-4 in solid form	59
31	Isotropic liquid of FZ-4 rapidly vaporized at 264.2°C	59
32	Smectic phase separating from isotropic phase of FZ-4 on first cooling at 262.3°C	60
33	Compound FZ-4 vapourized in the neighbourhood of deformation	60



	smectic phase	
34	IR Spectrum of FZ-49E, all the labeled peaks are representing stretching frequency of the appropriate functional groups, except for those mentioned other wise.	64
35	^1H NMR spectrum of FZ-49E (400 MHz, CDCl_3) (expanded)	65
36	^{13}C NMR spectrum of FZ-49E (400 MHz, CDCl_3)	66
37	DEPT spectrum of FZ-49E (100 MHz, CDCl_3)	67
38	DSC Thermogram of FZ-49E on second cooling and second heating	68
39	FZ-49E in solid form	69
40	Isotropic liquid of FZ-49E rapidly vaporized at 263°C	69
41	The natural mosaic texture of smectic phase separating from the isotropic liquid of FZ-49E on cooling at 147.2°C	70
42	The petal texture of smectic phase of FZ-49E at 145.2°C	70
43	IR Spectrum of FZ-37B, all the labeled peaks are representing stretching frequency of the appropriate functional groups, except for those mentioned other wise.	74
44	^1H NMR spectrum of FZ-37B (400 MHz, CDCl_3) (expanded)	75
45	^{13}C NMR spectrum of FZ-37B (400 MHz, CDCl_3)	76
46	DEPT spectrum of FZ-37B (100 MHz, CDCl_3)	77
47	DSC Thermogram of FZ-37B on second cooling and second heating	78



48	FZ-37B in solid form	79
49	Isotropic liquid of FZ-37B at 263°C	79
50	The spine texture of the smectic phase separating from the isotropic liquid of FZ-37B on cooling at 176.3°C; the black areas are homeotropic texture	80
51	The spine texture of smectic phase separating from the isotropic liquid of FZ-37B on cooling at 177.5°C	80
52	The spine texture of smectic phase separating from the isotropic liquid of FZ-49E on cooling at 176.5°C	81
53	The transition from spine texture of smectic phase to the faint band of crystalline phase of FZ-49E on cooling at 142.1°C	81
54	IR Spectrum of FZ-53, all the labeled peaks are representing stretching frequency of the appropriate functional groups, except for those mentioned other wise.	85
55	¹ H NMR spectrum of FZ-53 (400 MHz, CDCl ₃) (expanded)	86
56	¹³ C NMR spectrum of FZ-53 (400 MHz, CDCl ₃)	87
57	DEPT spectrum of FZ-53 (100 MHz, CDCl ₃)	88
58	DSC Thermogram of FZ-53 on second cooling and second heating	89
59	FZ-53 in solid form	90
60	Isotropic liquid of FZ-53 at 183°C	90
61	The separation of the smectic phase in the form of droplet from isotropic liquid of FZ-53 on second cooling at 169.1°C	91
62	The broken fan-shaped textures of smectic phase of FZ-53 on second	91



	cooling at 168°C	
63	The single fan of smectic phase of FZ-53	92
64	The smectic phase colour rearrangement of FZ-53	92
65	The transition from broken fan-shaped texture of smectic phase to the banded crystalline phase texture of FZ-49E on cooling at 145.7°C	93
66	The banded crystalline phase of FZ-53	93
67	IR Spectrum of FZ-34A, all the labeled peaks are representing stretching frequency of the appropriate functional groups, except for those mentioned other wise.	97
68	¹ H NMR spectrum of FZ-34A (400 MHz, CDCl ₃) (expanded)	98
69	¹³ C NMR spectrum of FZ-34A (400 MHz, CDCl ₃)	99
70	DEPT spectrum of FZ-34A (100 MHz, CDCl ₃)	100
71	DSC Thermogram of FZ-34A on second cooling and second heating	101
72	FZ-34A in solid form	102
73	Isotropic liquid of FZ-34A at 175°C	103
74	The broken fan-shaped texture of smectic phase formed on cooling isotropic liquid of FZ-34A at 169.3°C	103
75	The smectic phase colour rearrangement of FZ-34A	102
76	The transition from broken fan-shaped texture of smectic phase to the banded crystalline phase texture of FZ-34A on cooling at 139.2°C	104
77	The banded crystalline phase of FZ-34A	104
78	IR Spectrum of FZ-35A, all the labeled peaks are representing stretching frequency of the appropriate functional groups, except for	107



those mentioned other wise.

79	¹ H NMR spectrum of FZ-35A (400 MHz, CDCl ₃) (expanded)	108
80	¹³ C NMR spectrum of FZ-35A (400 MHz, CDCl ₃)	109
81	DEPT spectrum of FZ-35A (100 MHz, CDCl ₃)	110
82	DSC Thermogram of FZ-35A on second cooling and second heating	111
83	FZ-35A in solid form	112
84	Isotropic liquid of FZ-35A at 170°C	112
85	The sanded texture of smectic phase of FZ-35A on second heating at 150°C	113
86	The natural <i>schlieren</i> texture of smectic phase FZ-35A on second cooling at 155°C	113
87	The phase transition to the <i>schlieren</i> nematic texture of the smectic phase on second heating at 145°C	114
88	The <i>schlieren</i> texture of the nematic phase formed on cooling the homeotropic texture of smectic phase of FZ-35A on second cooling at 163°C. The texture exhibits centres of four <i>schlieren</i>	114
89	The transition phase from nematic phase to the crystalline phase of FZ-35A on cooling at 131.2°C	115
90	The crystalline phase of FZ-35A	115



LIST OF ABBREVIATIONS

LCs	Liquid Crystals
S	Smectic
N	Nematic
DSC	Differential Scanning Calorimetry
OPM	Optical Polarize Microscope
DCC	1,3-dicyclohexylcarbodiimide
DMAP	4-(N,N-dimethylamino)pyridine
POMBOH	2-(prenyloxymethyl)benzoic acid
POMB	2-(prenyloxymethyl)benzoyl
CH ₂ Cl ₂	dichloromethane
NaOH	Natrium hydroxide
¹ H	proton
¹³ C	Carbon 13
NMR	Nuclear Magnetic Resonance
DEPT	Distortionless Enhancement by Polarisation Transfer
IR	Infra red
EIMS	Electron Impact Mass Spectrometry
CDCl ₃	chloroform
DMSO- <i>d</i> ₆	dimethyl sulfoxide
cm ⁻¹	per centimeter
°C	degree in Celcius



δ	delta (chemical shift in ppm)
g	gram
m.p.	melting point
R	Alkyl group
I	Isotropic
Cr	Crystalline
d	doublet
dd	doublet of doublet
t	triplet
s	singlet
m	multiplet

