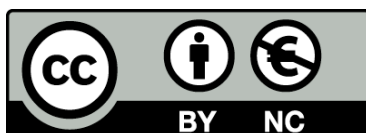




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Alquenos altamente piramidalizados funcionalizados: generación, transformaciones y estudios relacionados

M^a Rosa Muñoz Blasco



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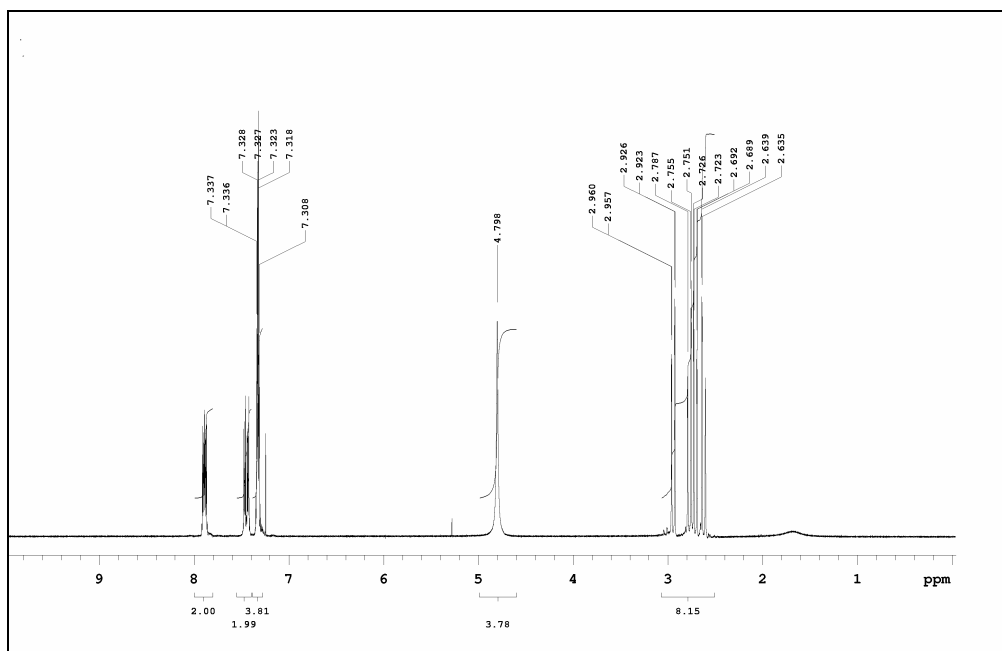
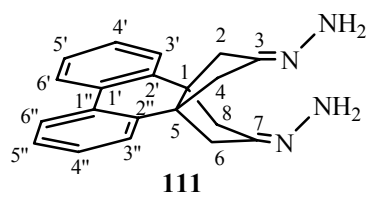
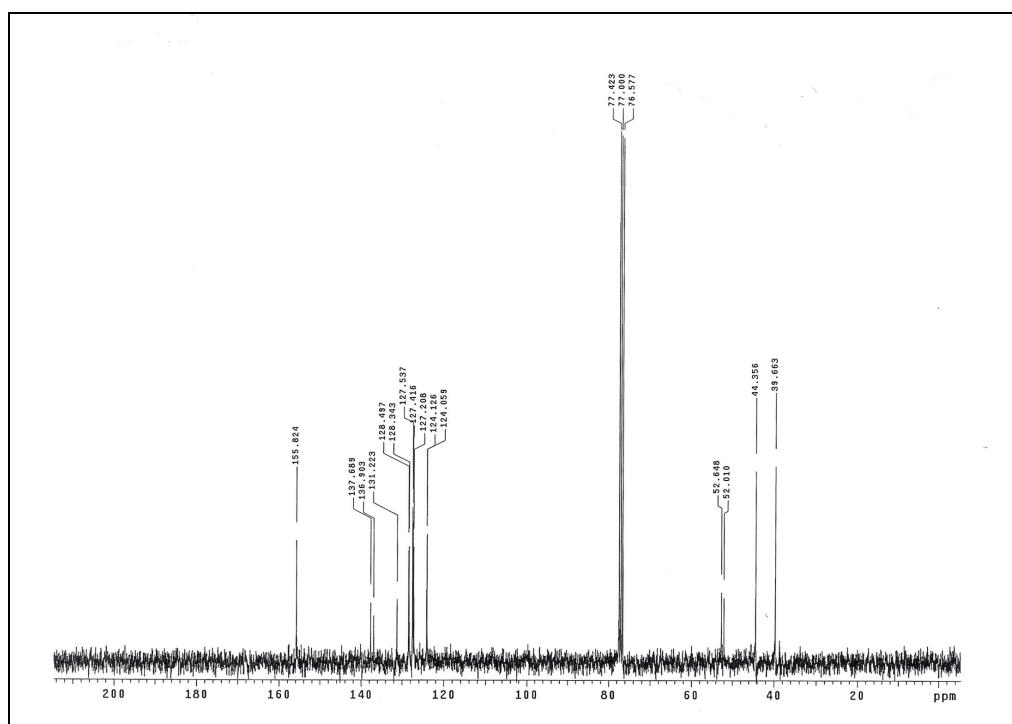
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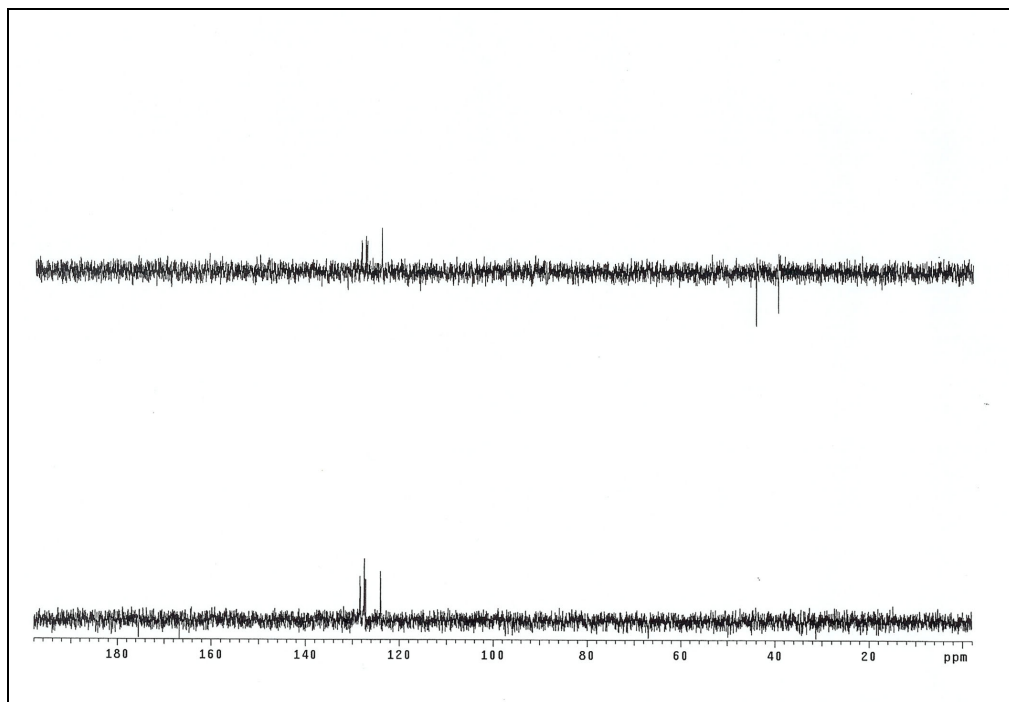
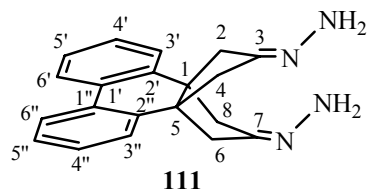
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Anexo Espectroscópico

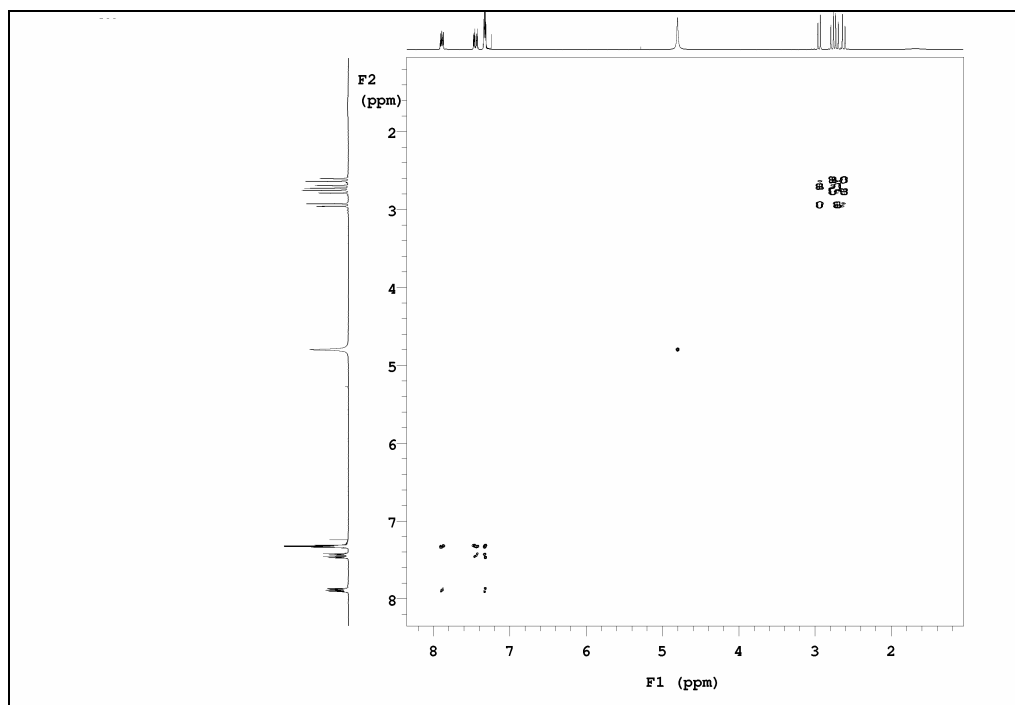
Anexo 1.

Espectros de ^1H , ^{13}C , DEPT, homocorrelaciones, heterocorrelaciones y IR

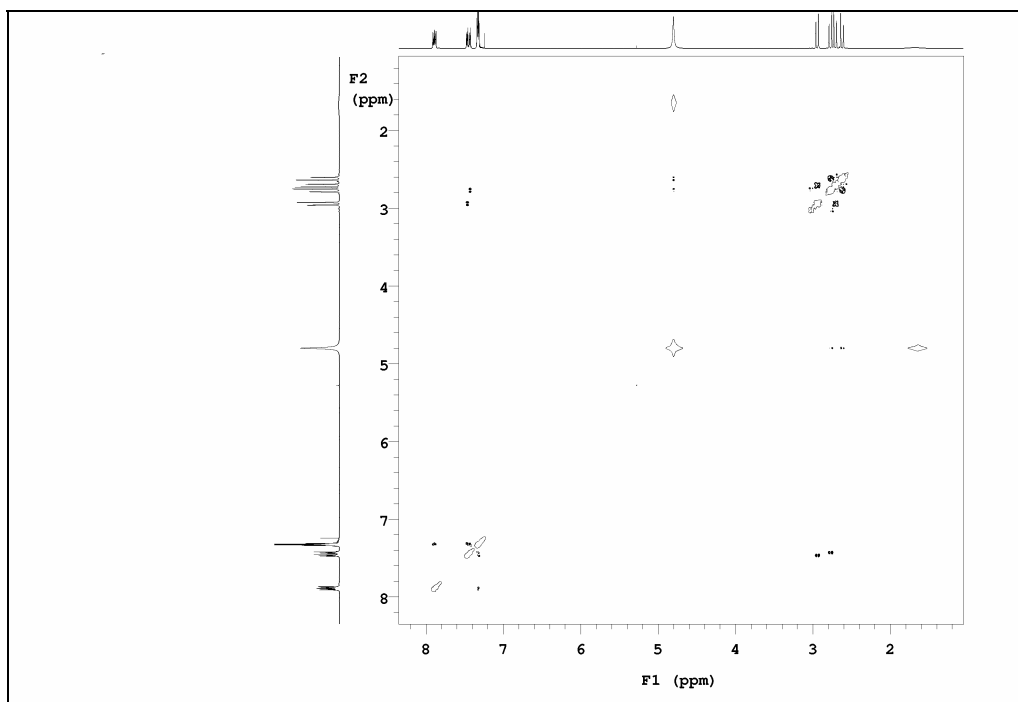
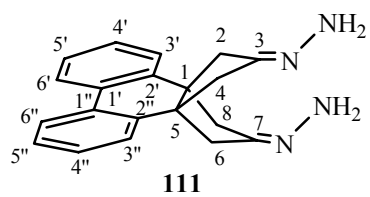
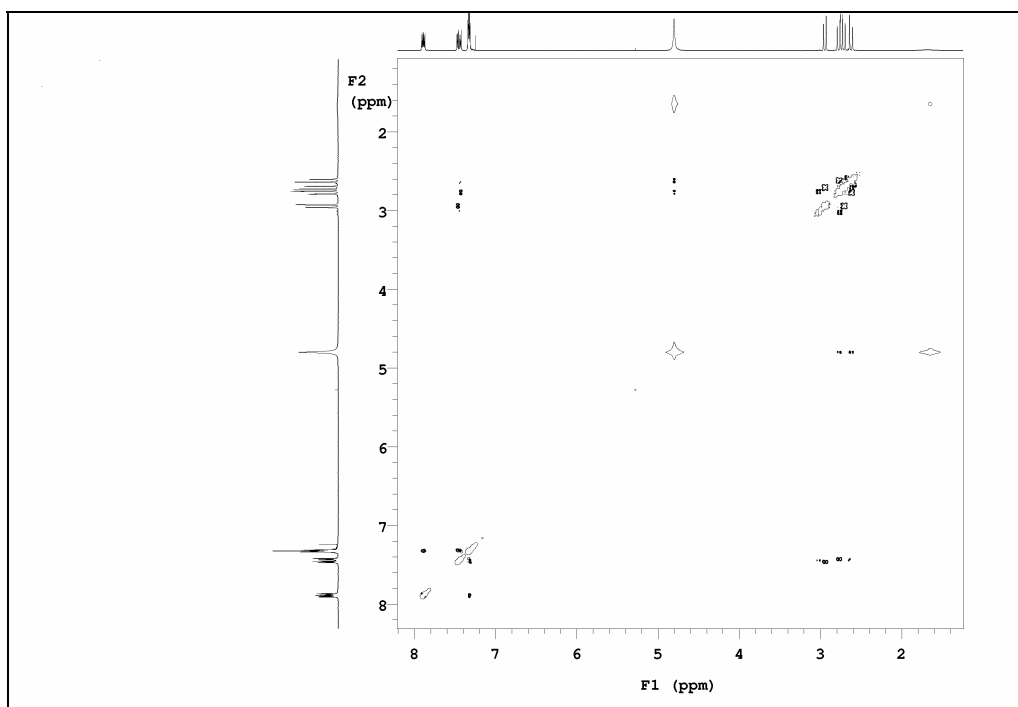
 $^1\text{H-RMN}$ (500 MHz, CDCl_3) $^{13}\text{C-RMN}$ (75.4 MHz, CDCl_3)

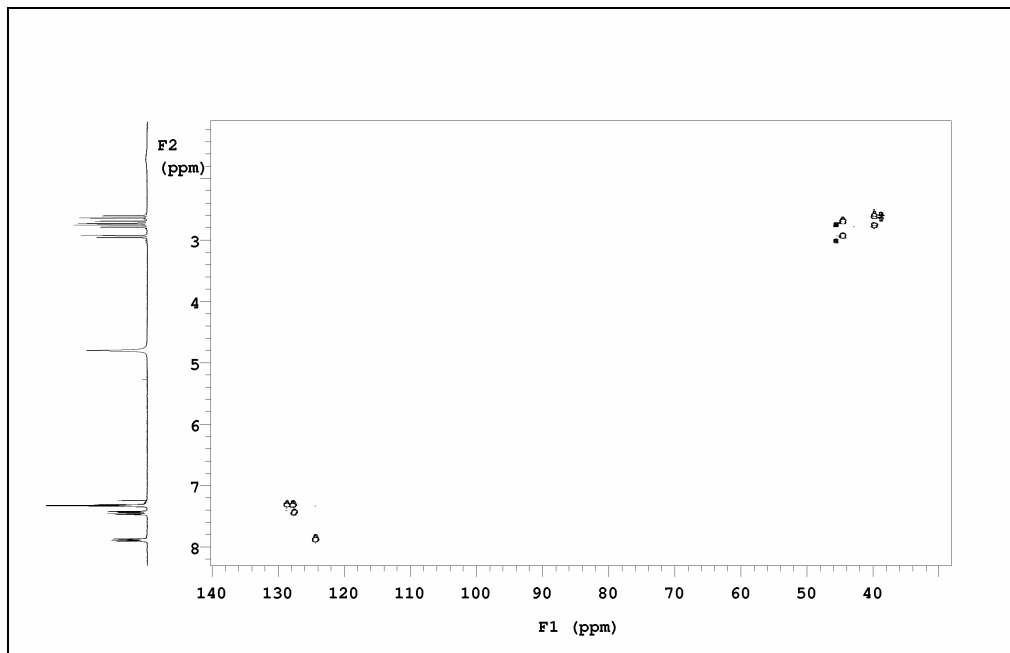
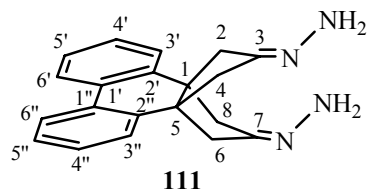


¹³C-DEPT

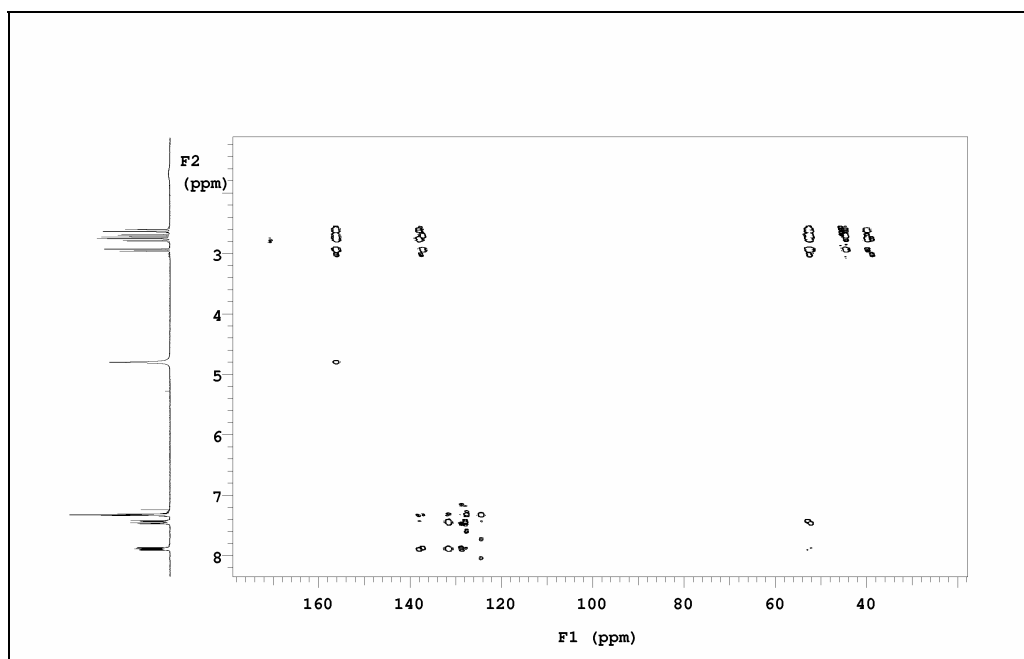


¹H-¹H-COSY

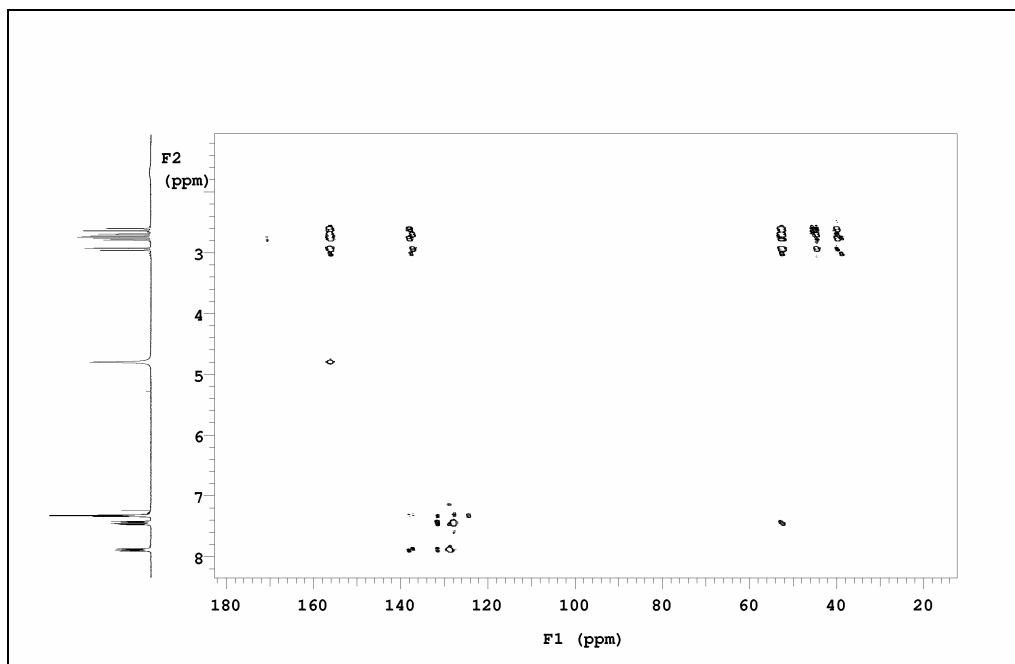
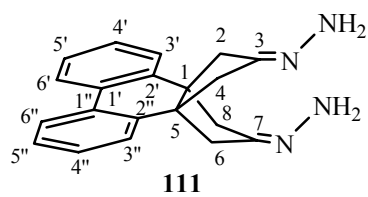
 ^1H - ^1H -NOESY 0.5 ^1H - ^1H -NOESY 0.8



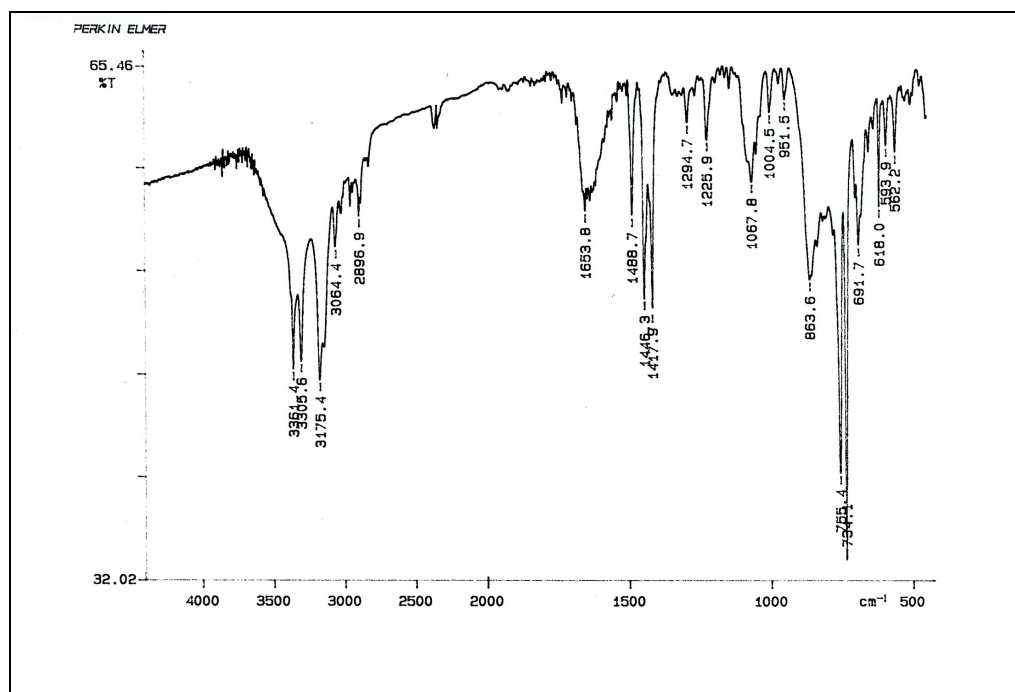
$^1\text{H}-^{13}\text{C}$ -HSQC



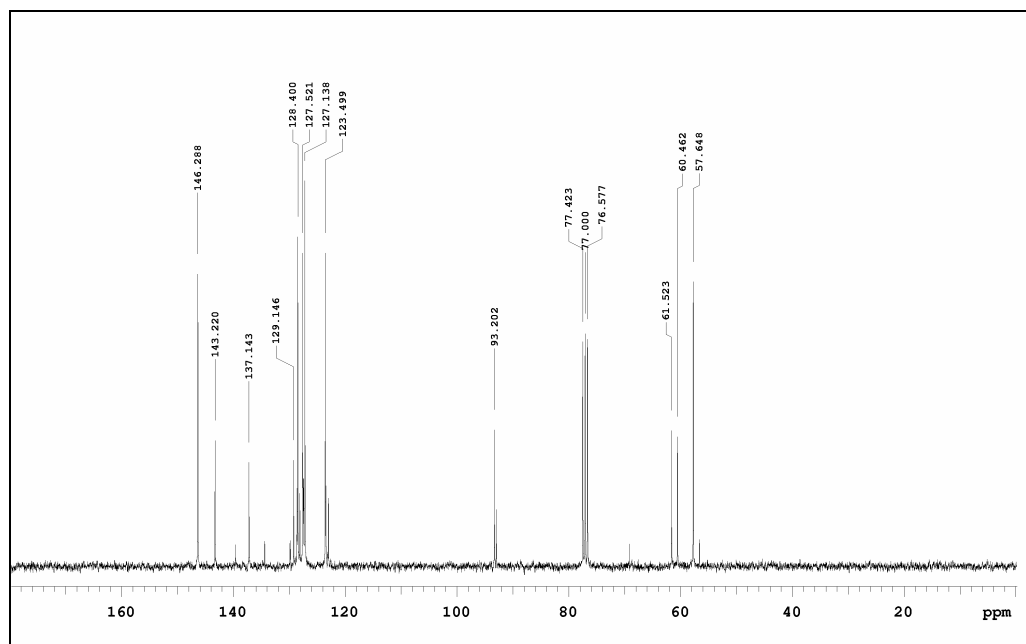
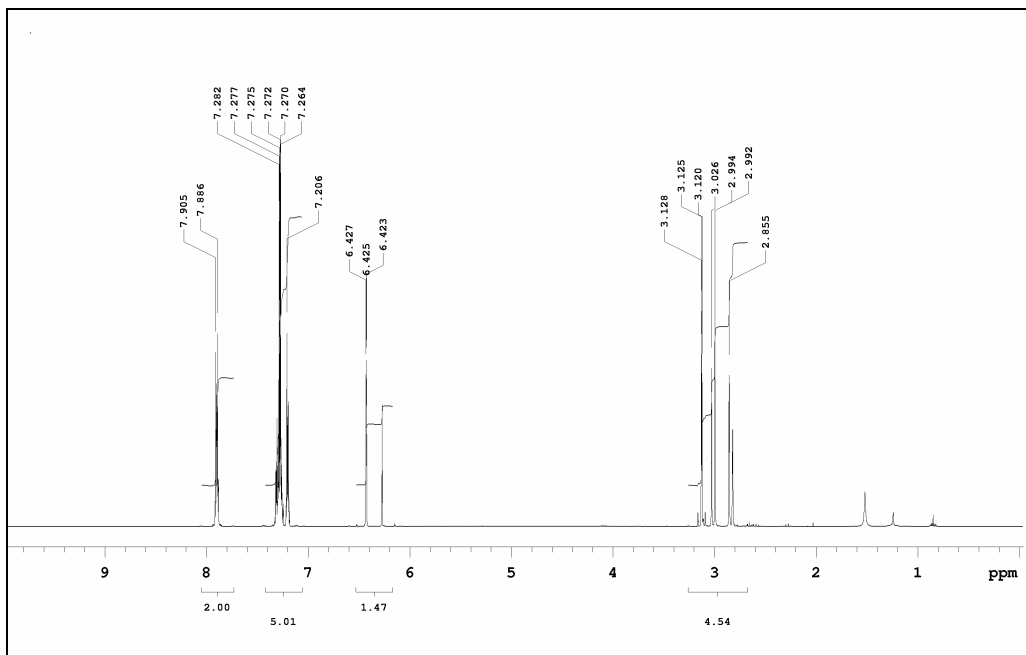
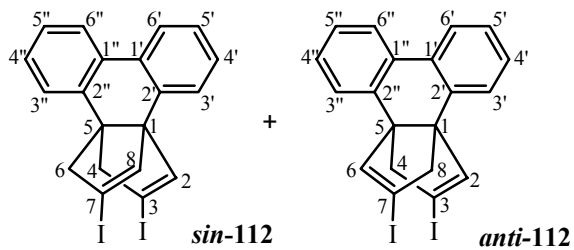
$^1\text{H}-^{13}\text{C}$ -HMBC $J=5$ Hz

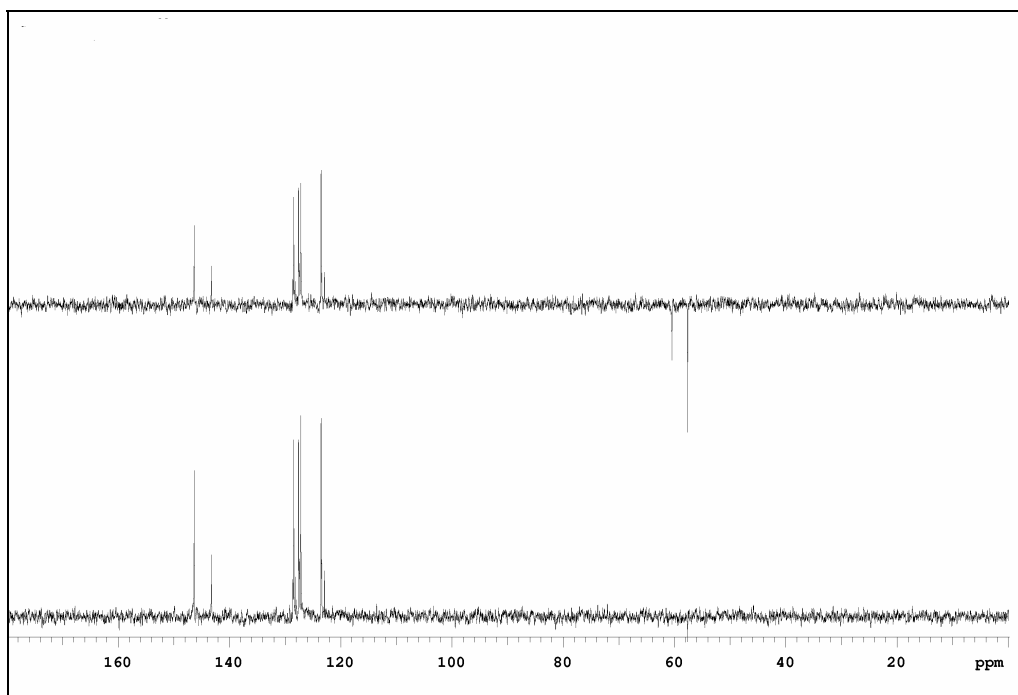
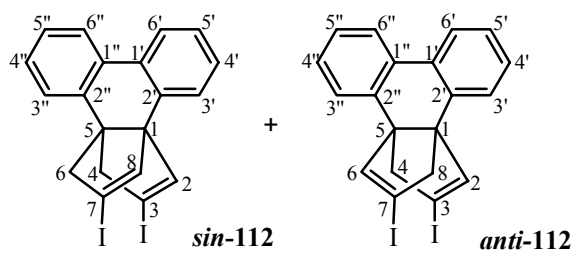


$^1\text{H}-^{13}\text{C}$ -HMBC $J=8$ Hz

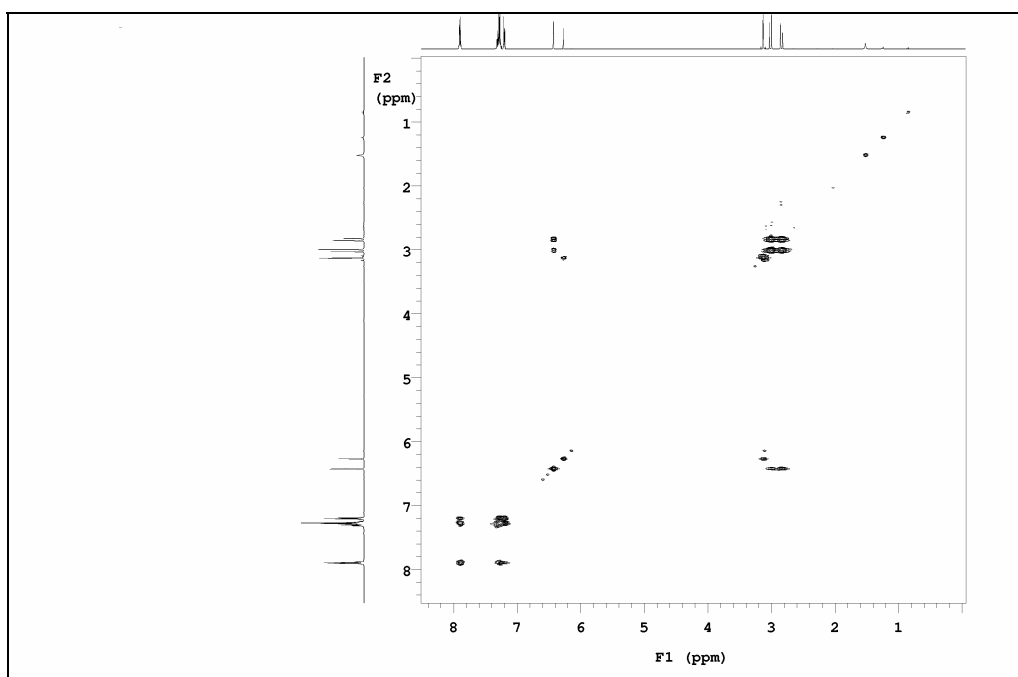


IR (KBr)

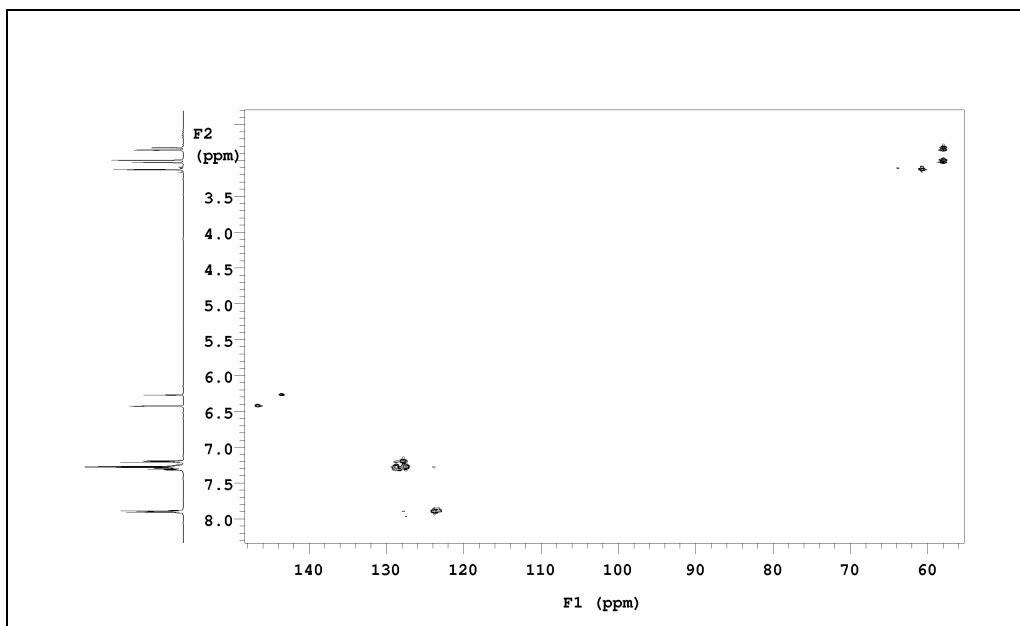
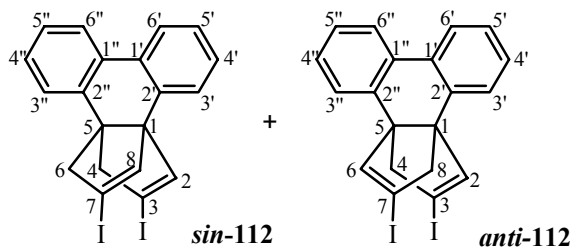




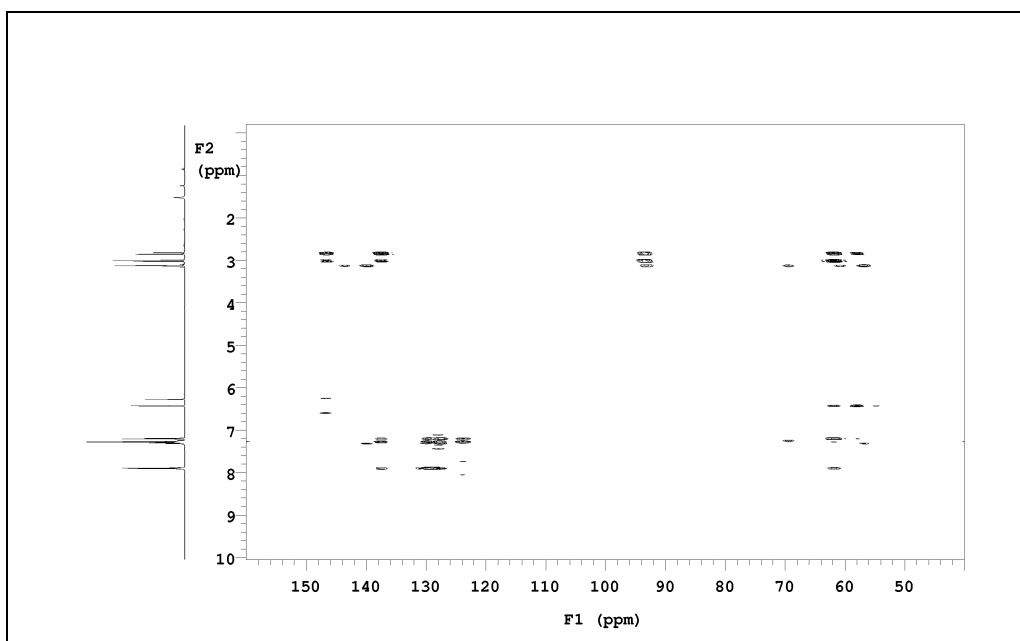
$^{13}\text{C-DEPT}$



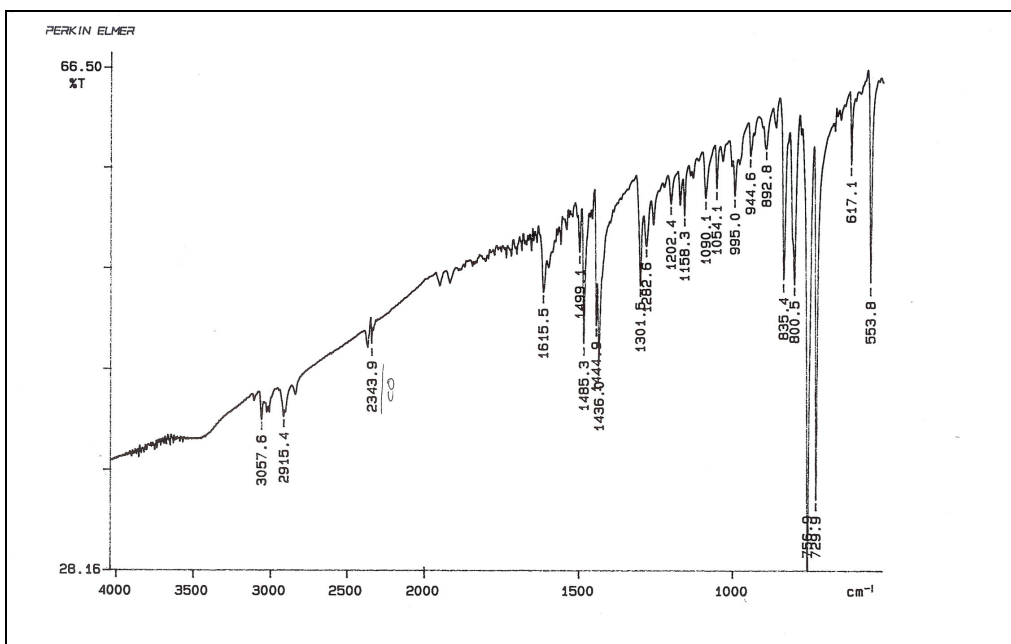
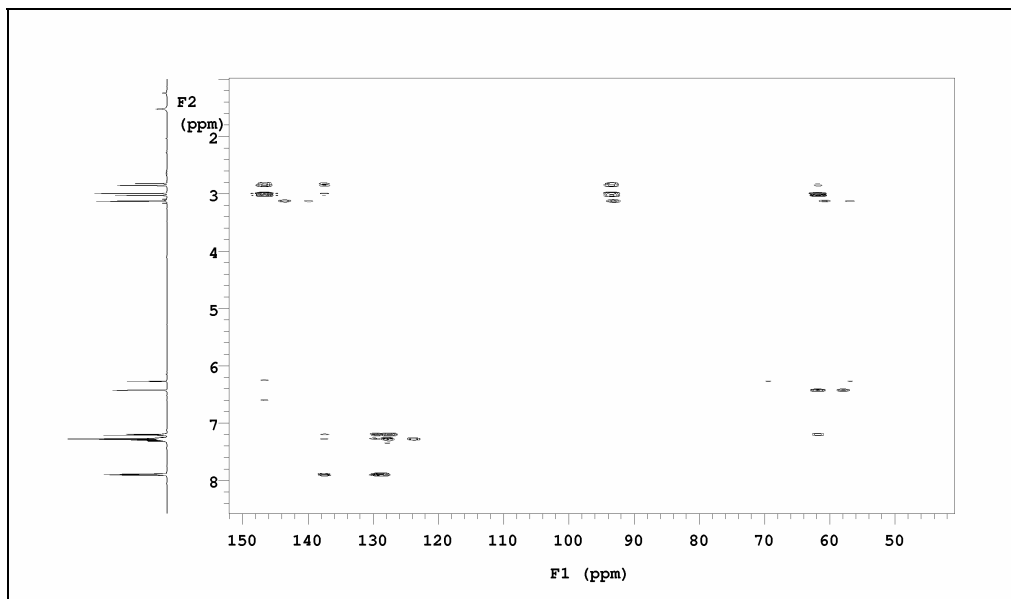
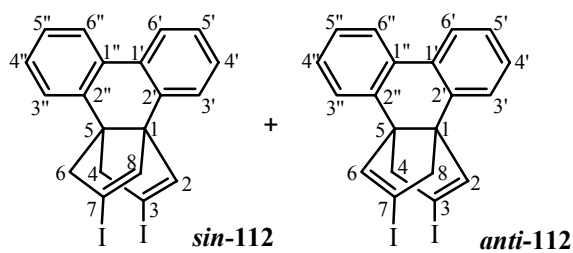
$^1\text{H-}^1\text{H-COSY}$

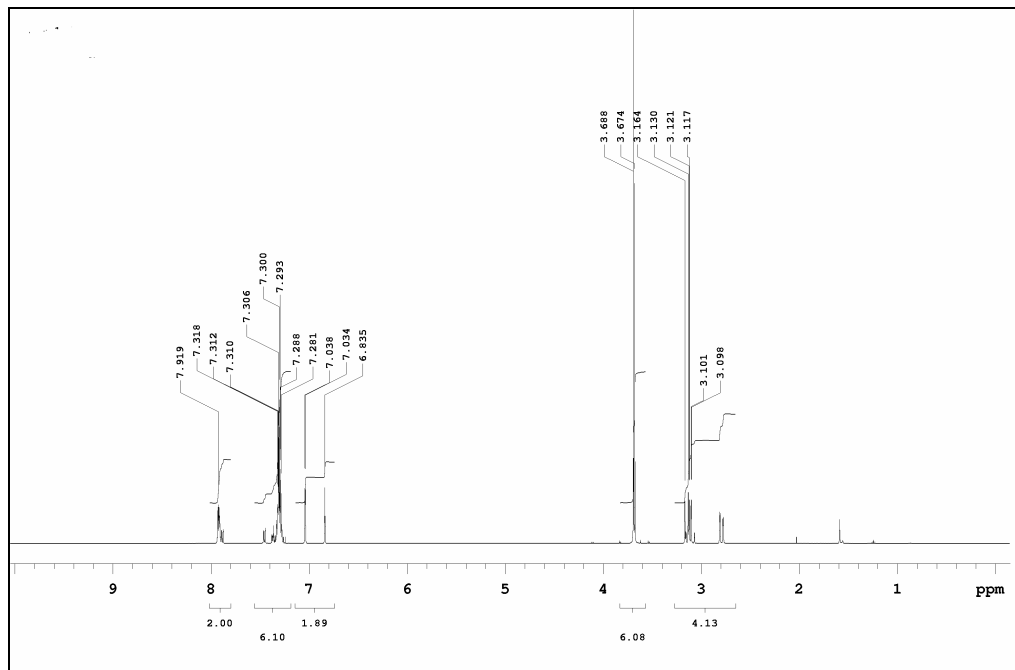
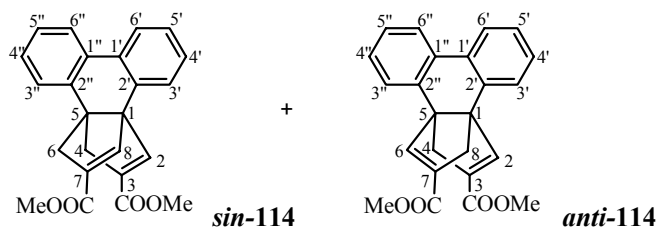


$^1\text{H}-^{13}\text{C}$ -HSQC

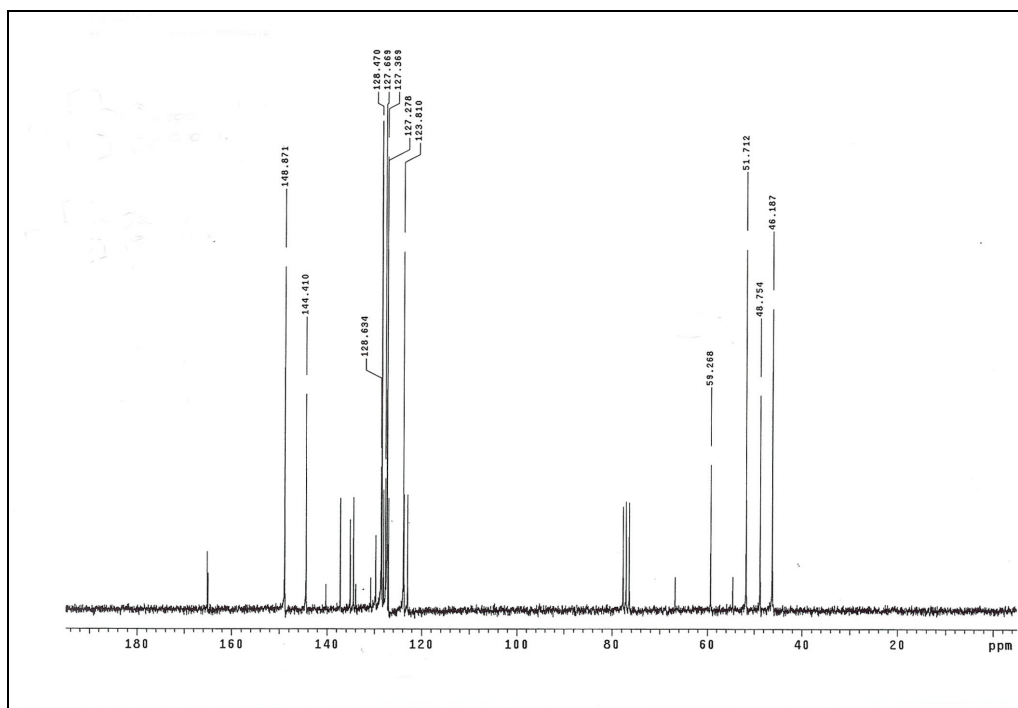


$^1\text{H}-^{13}\text{C}$ -HMBC $J = 3 \text{ Hz}$

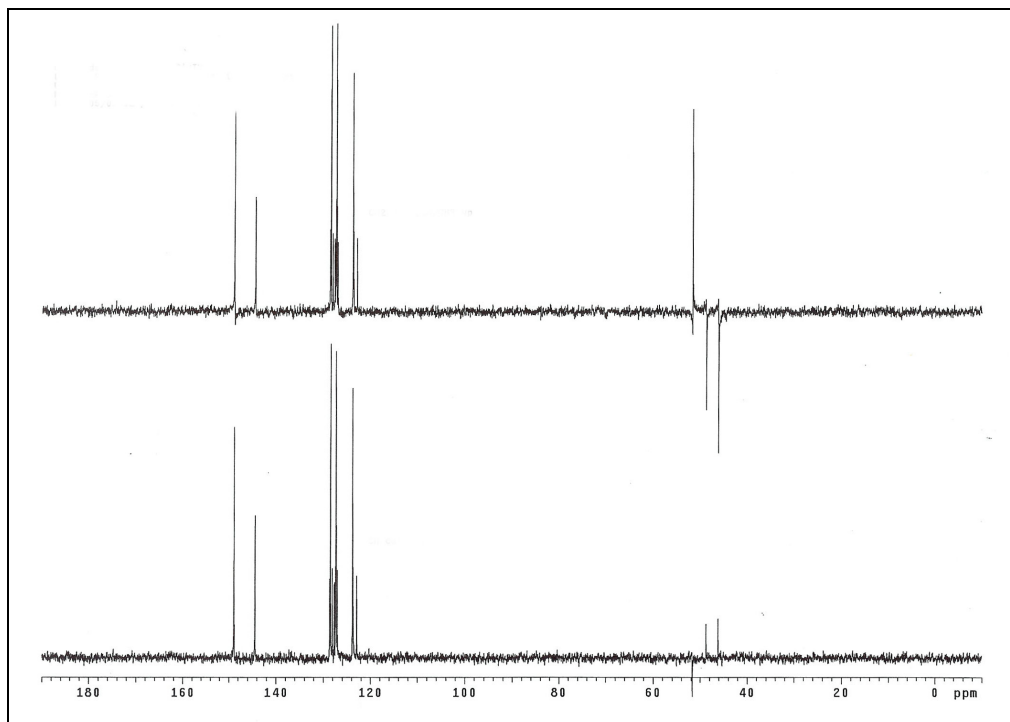
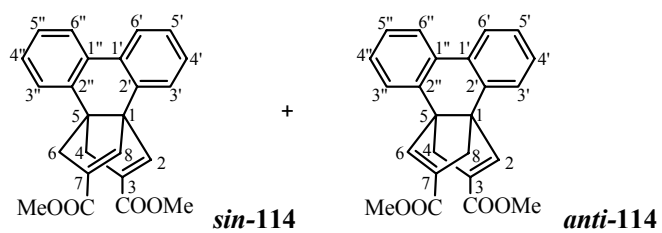
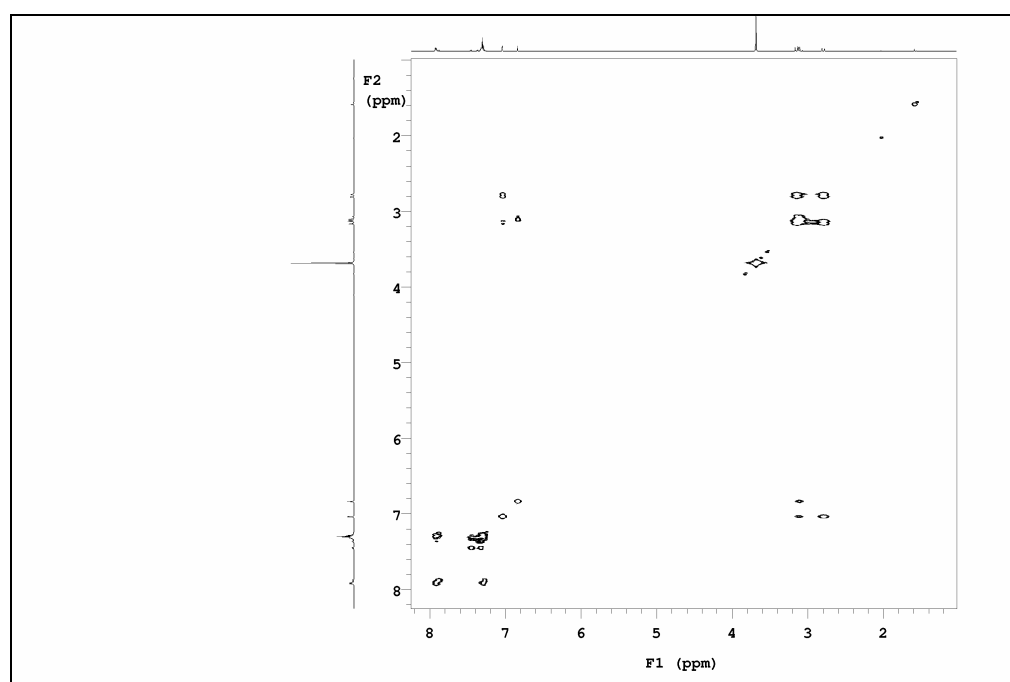


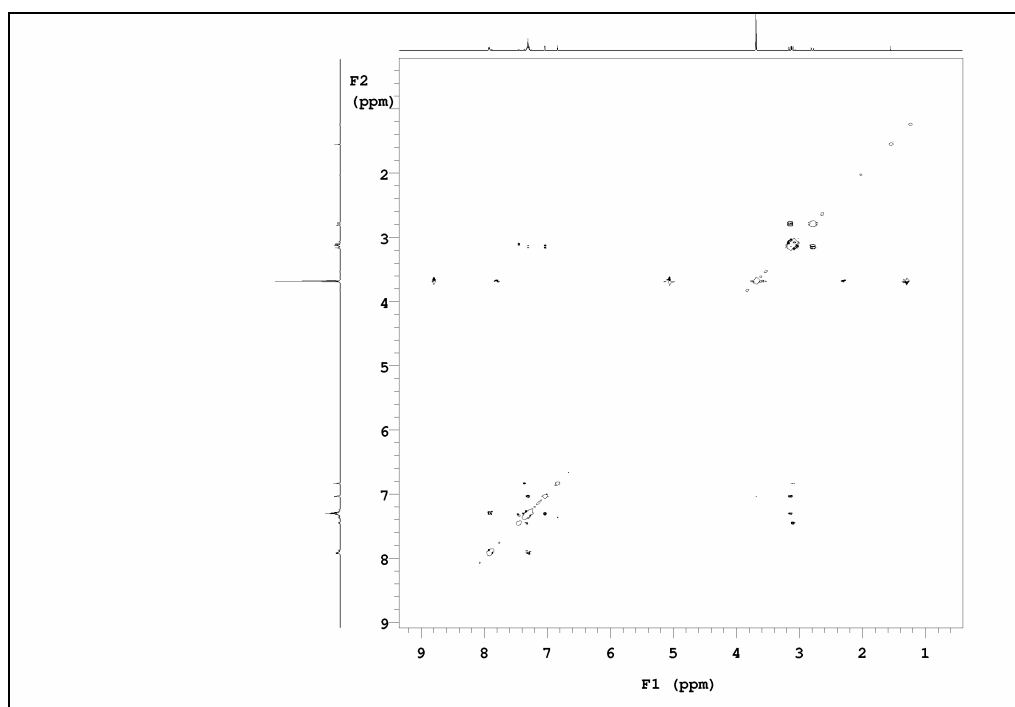
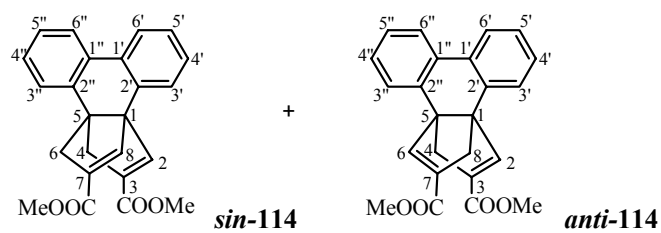


$^1\text{H-RMN}$ (500 MHz, CDCl_3)

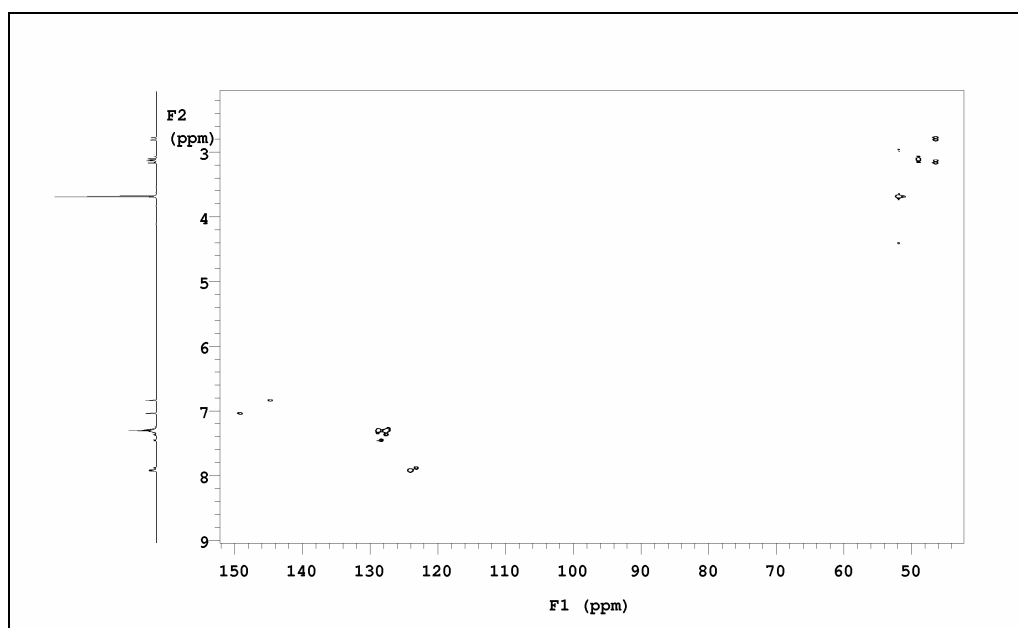


$^{13}\text{C-RMN}$ (50.3 MHz, CDCl_3)

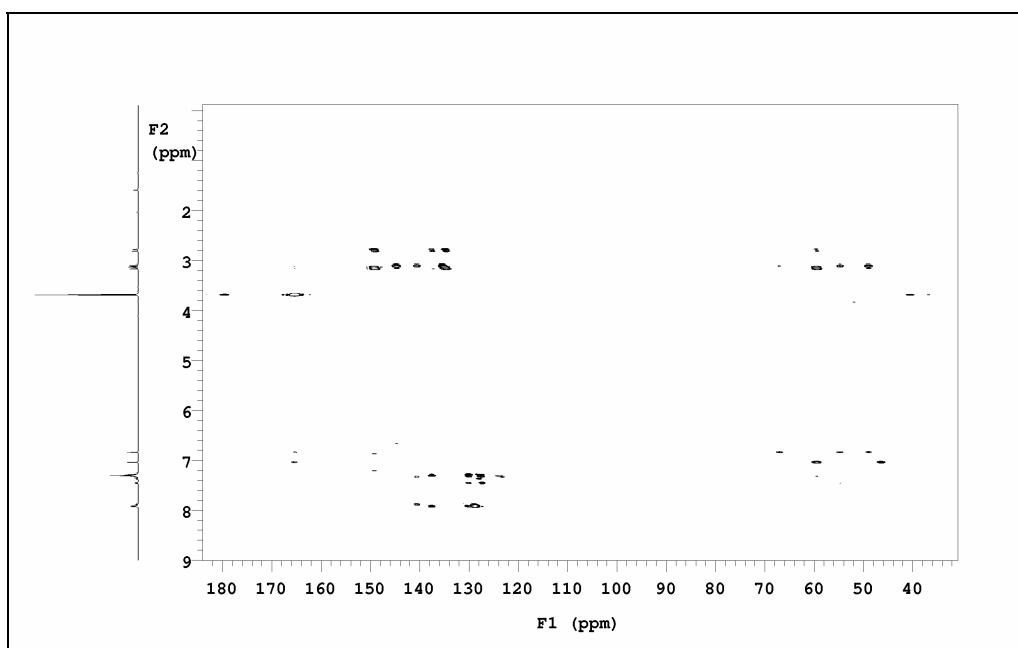
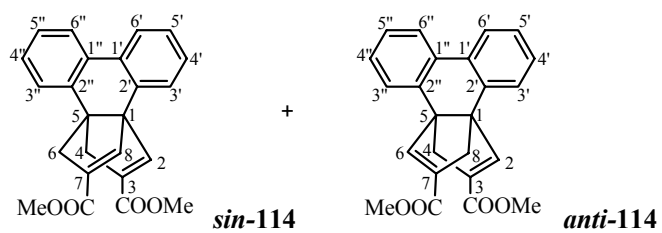
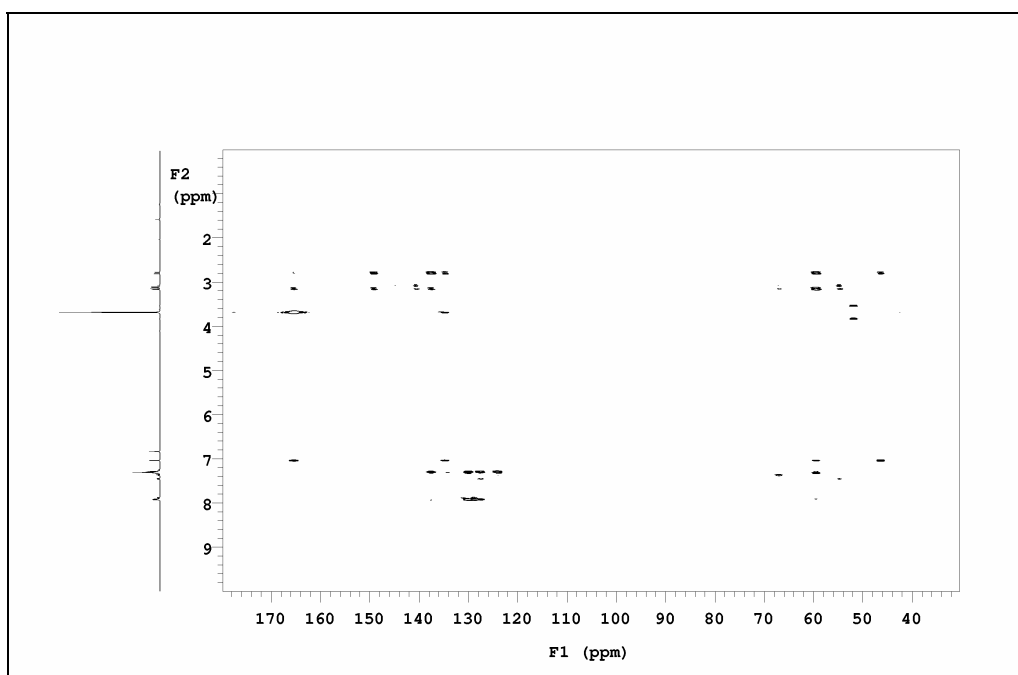
 ^{13}C -DEPT ^1H - ^1H -COSY

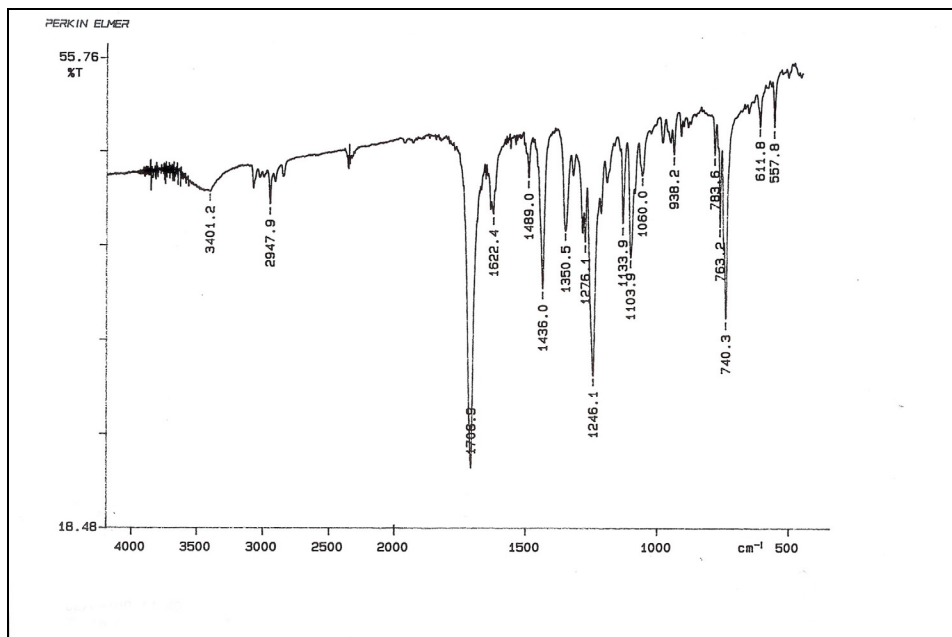
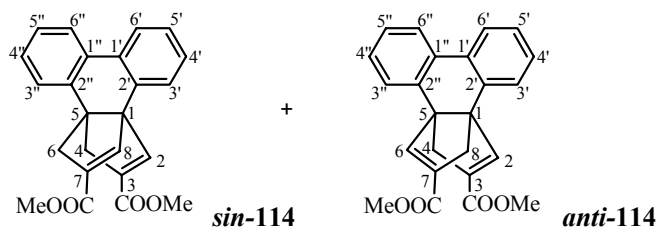


^1H - ^1H -NOESY

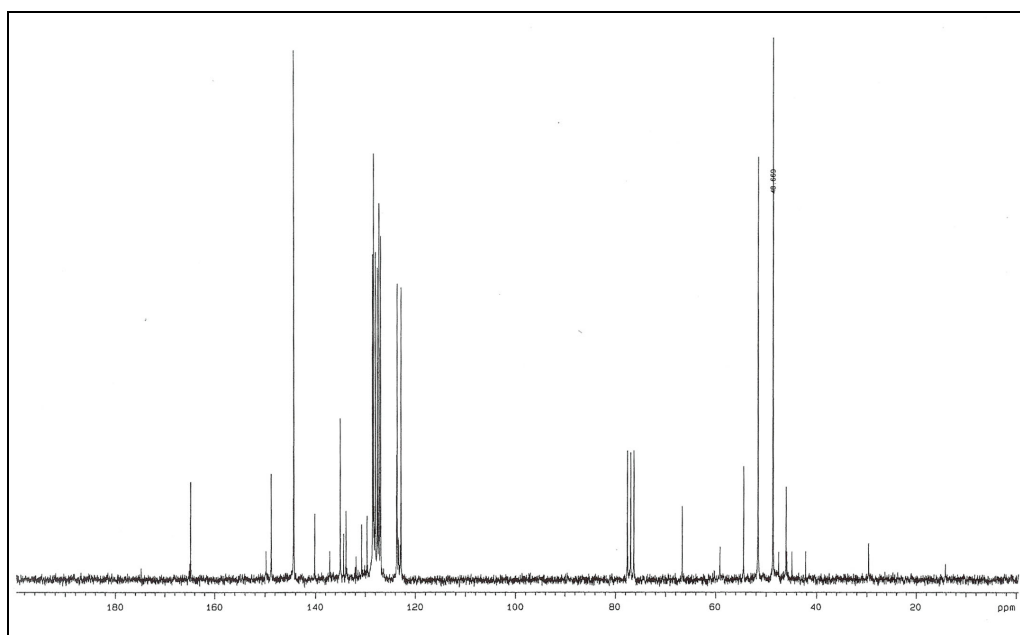
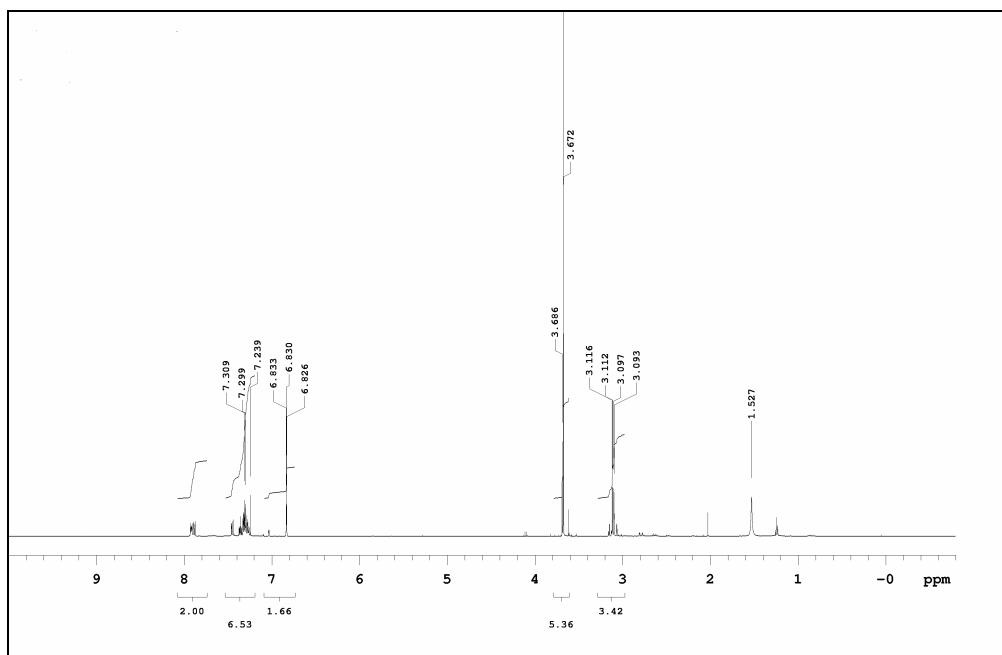
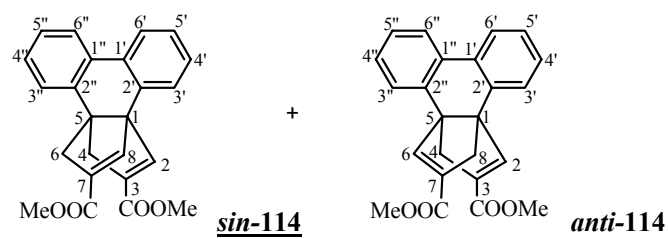


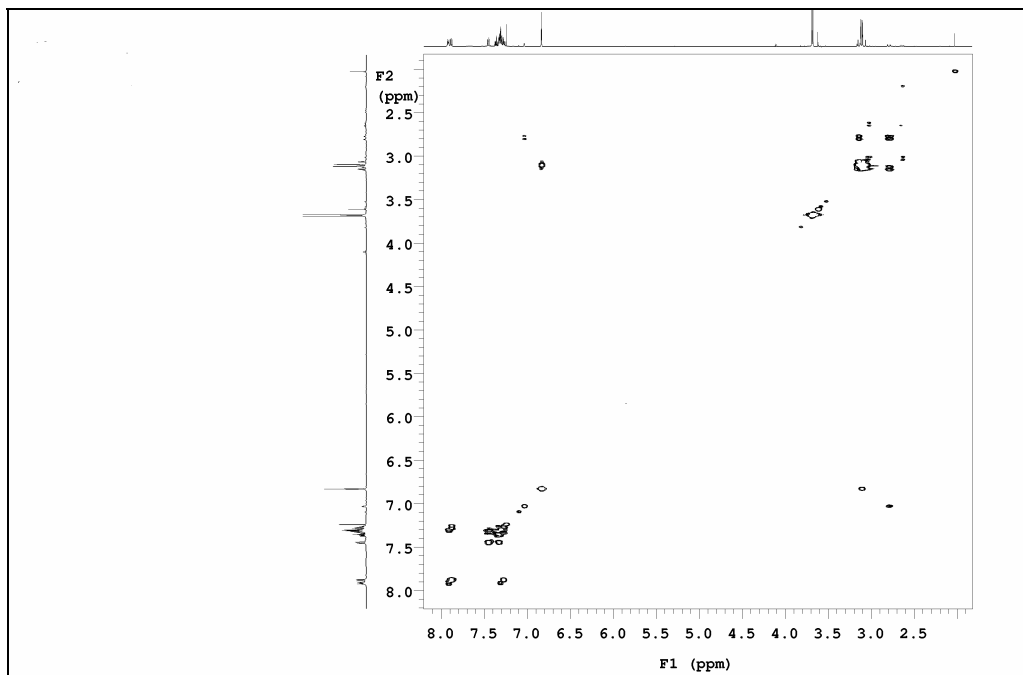
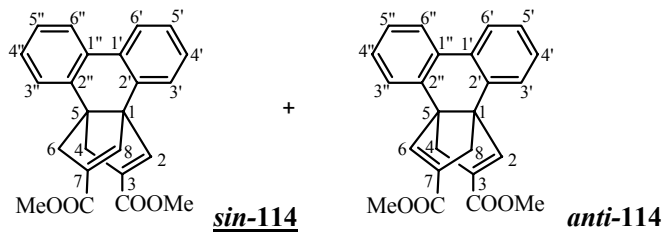
^1H - ^{13}C -HSQC

 $^1\text{H}-^{13}\text{C}\text{-HMBC } J = 8 \text{ Hz}$  $^1\text{H}-^{13}\text{C}\text{-HMBC } J = 3 \text{ Hz}$

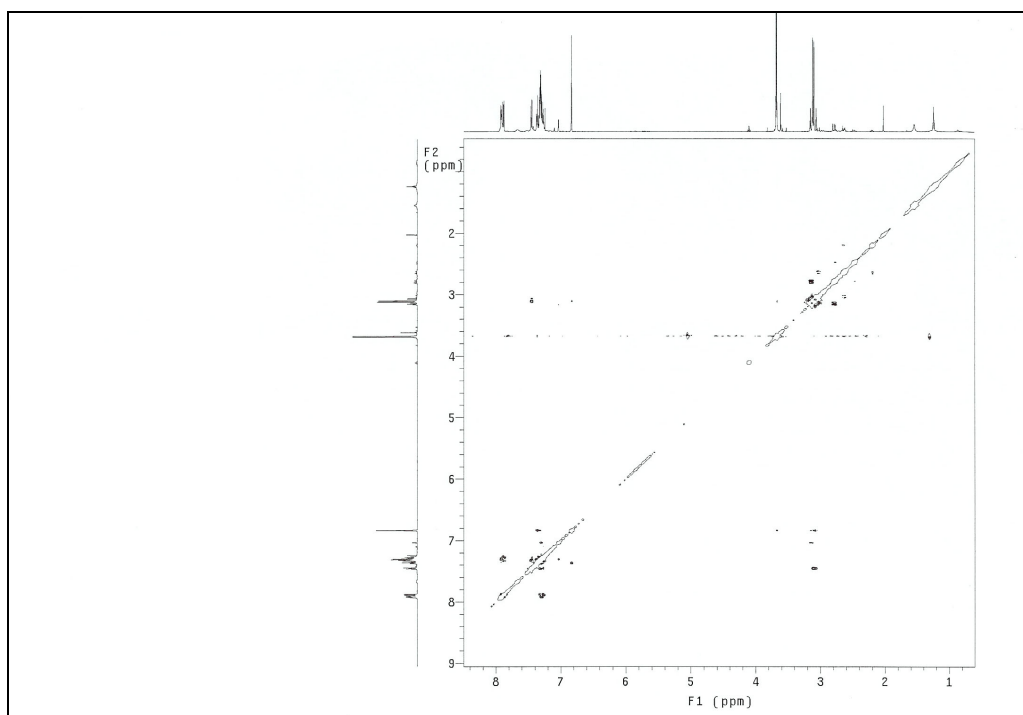


IR (KBr)

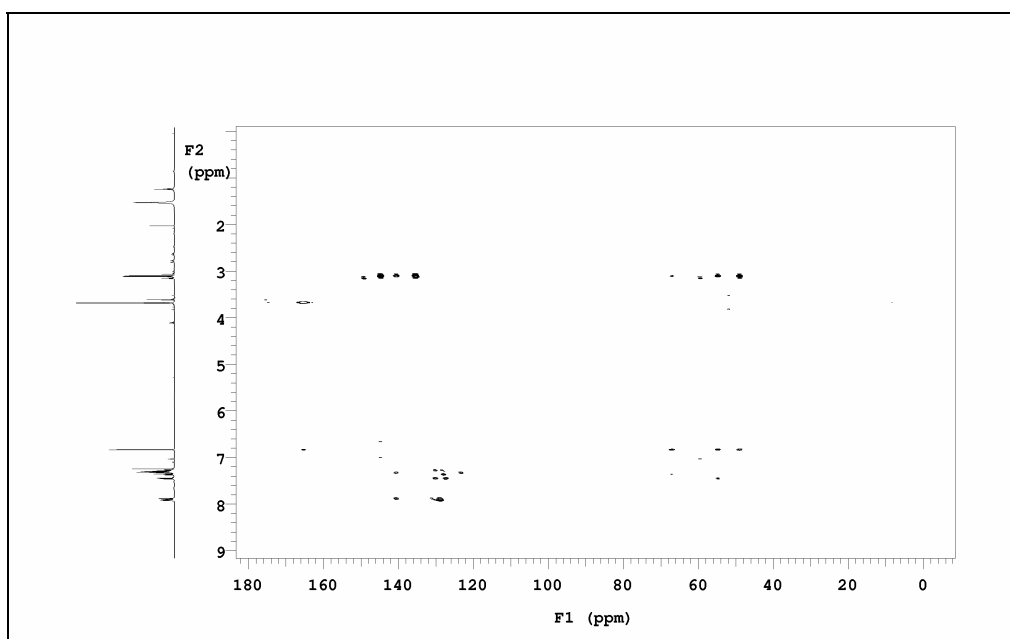
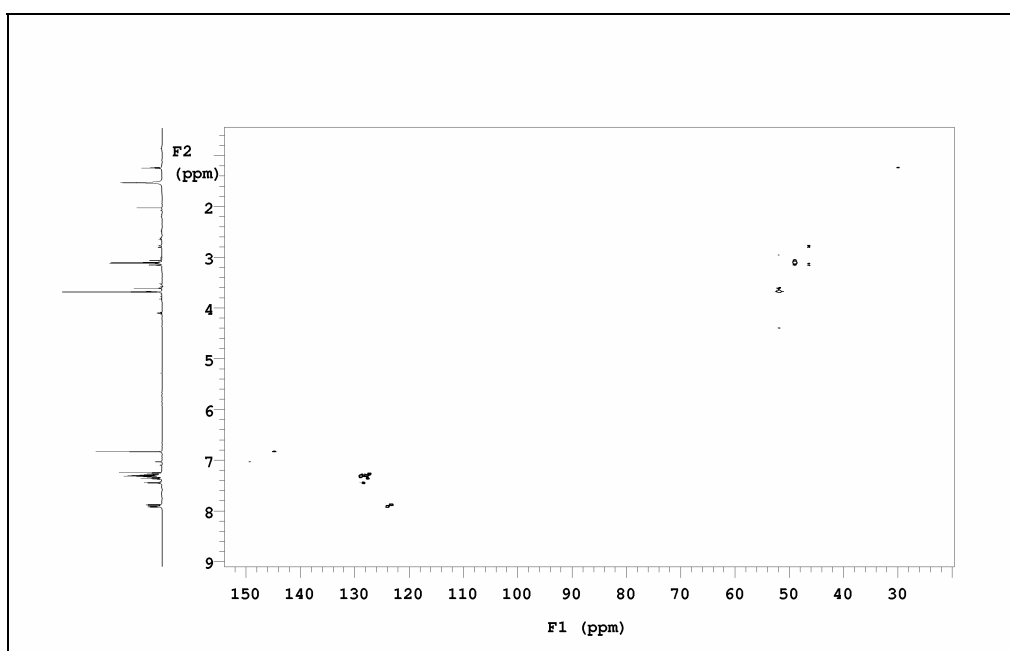
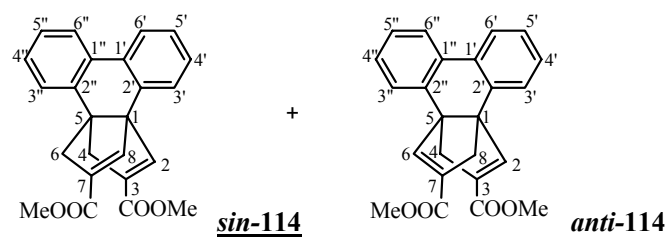


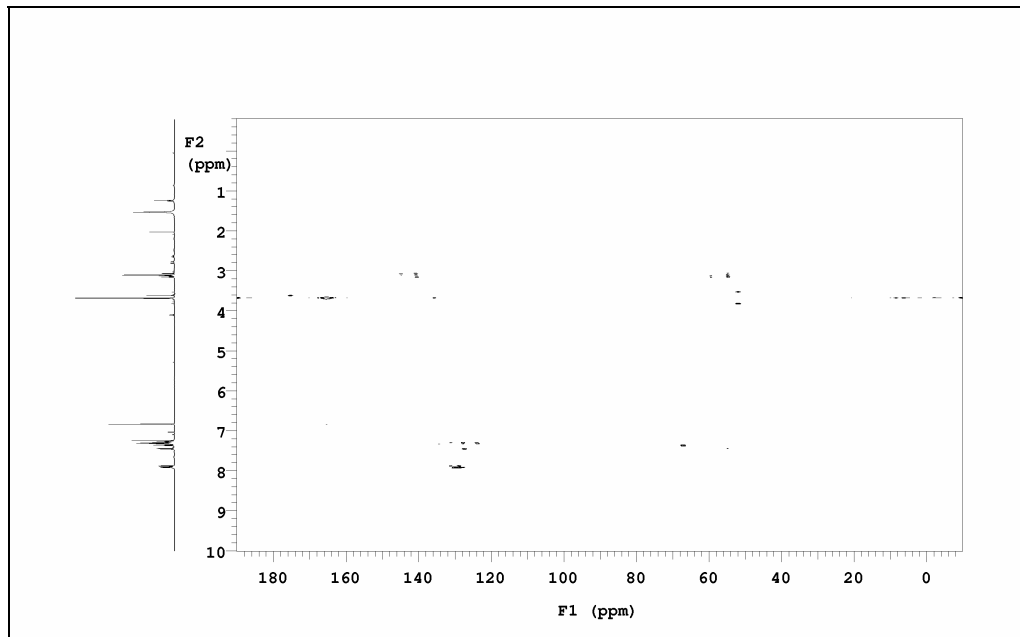
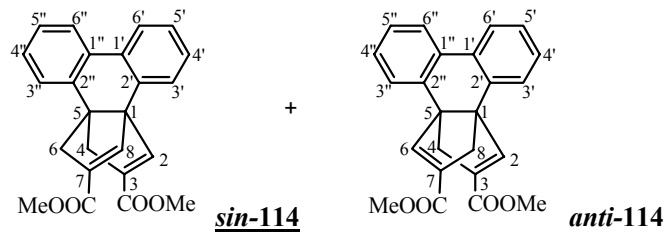


$^1\text{H}-^1\text{H}$ -COSY

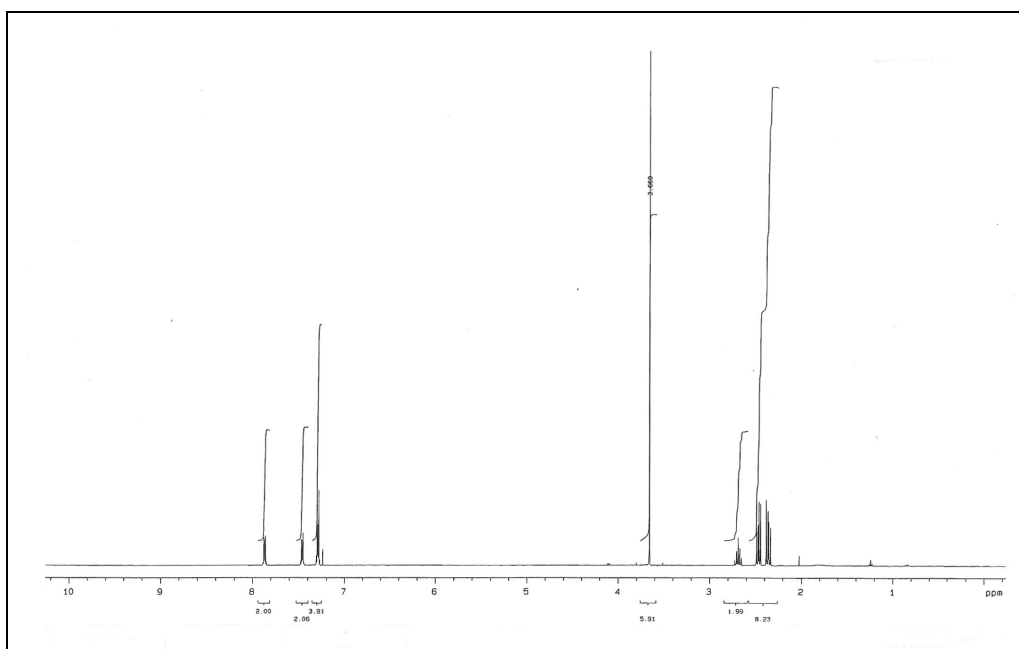
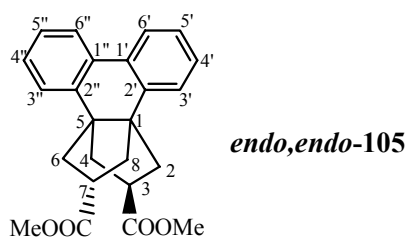
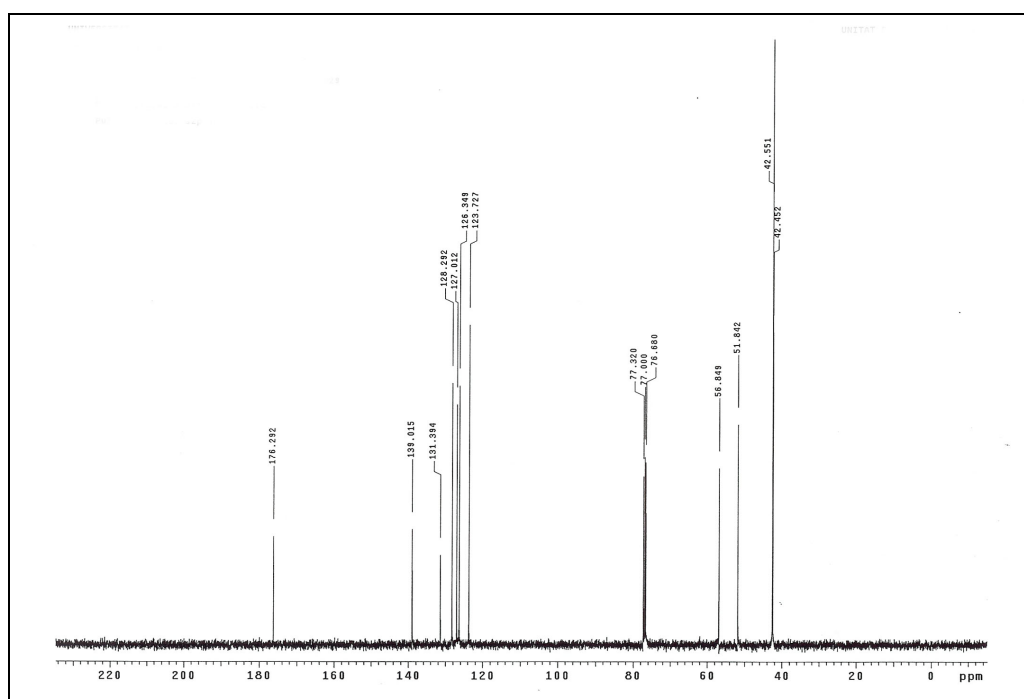


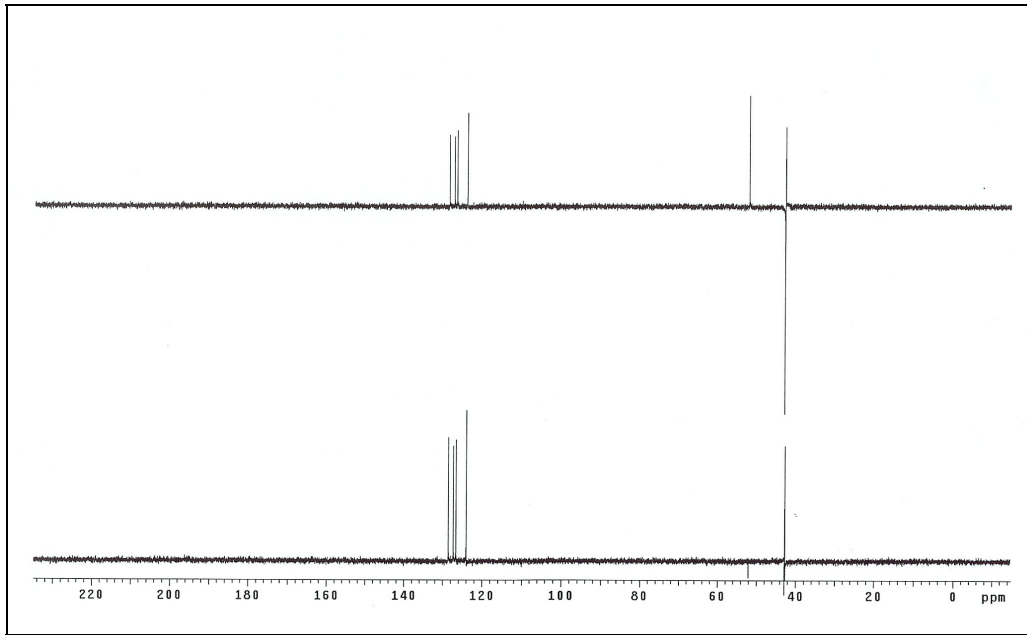
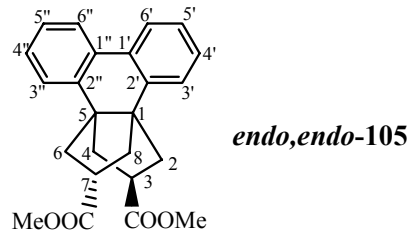
$^1\text{H}-^1\text{H}$ -NOESY



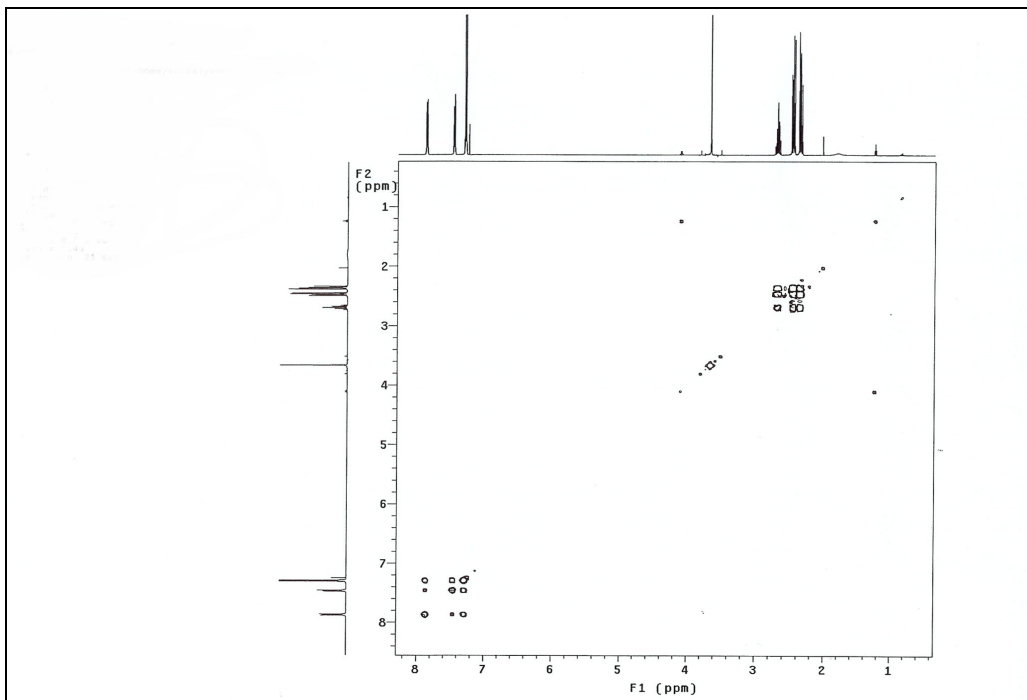


$^1\text{H}-^{13}\text{C}$ -HMBC $J=3\text{ Hz}$

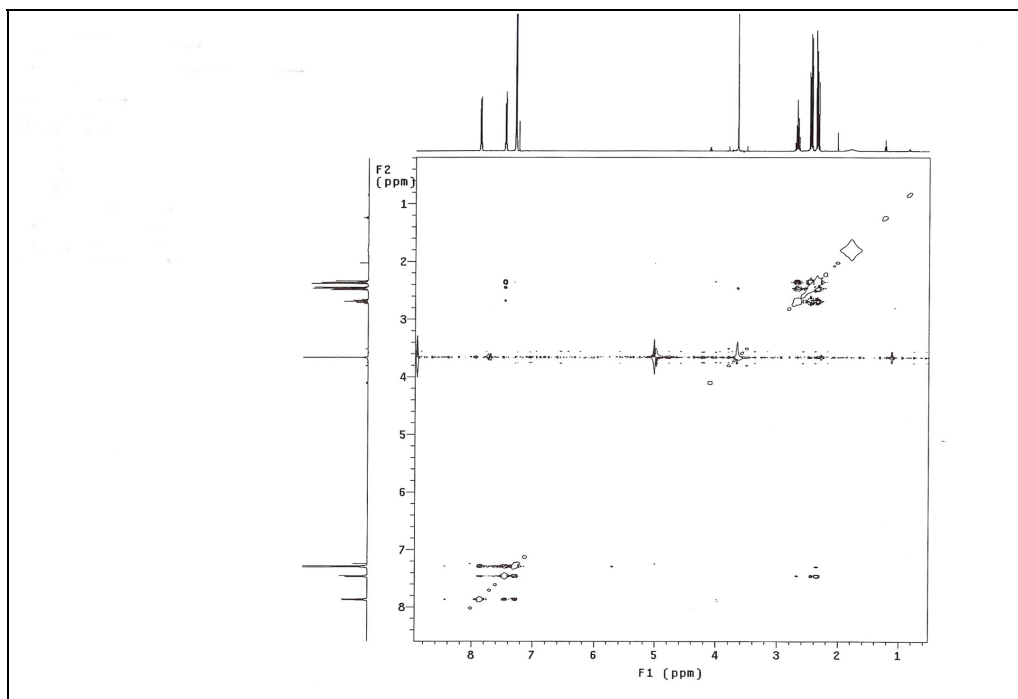
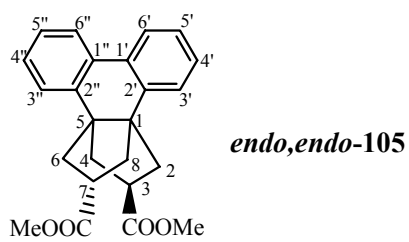
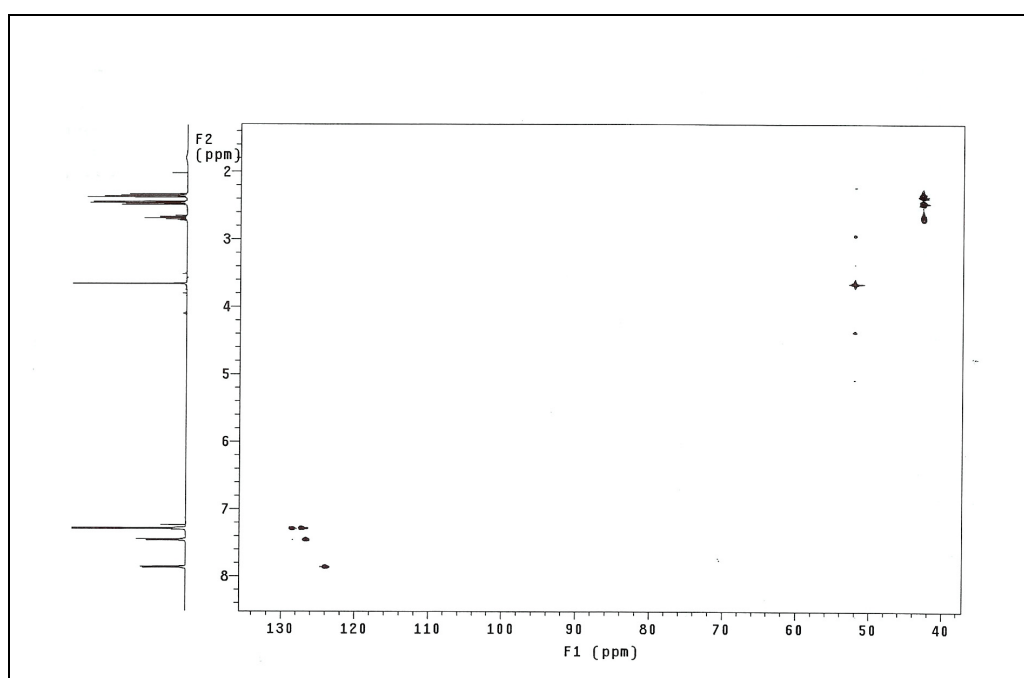
 $^1\text{H-RMN}$ (500 MHz, CDCl_3) $^{13}\text{C-RMN}$ (100.6 MHz, CDCl_3)

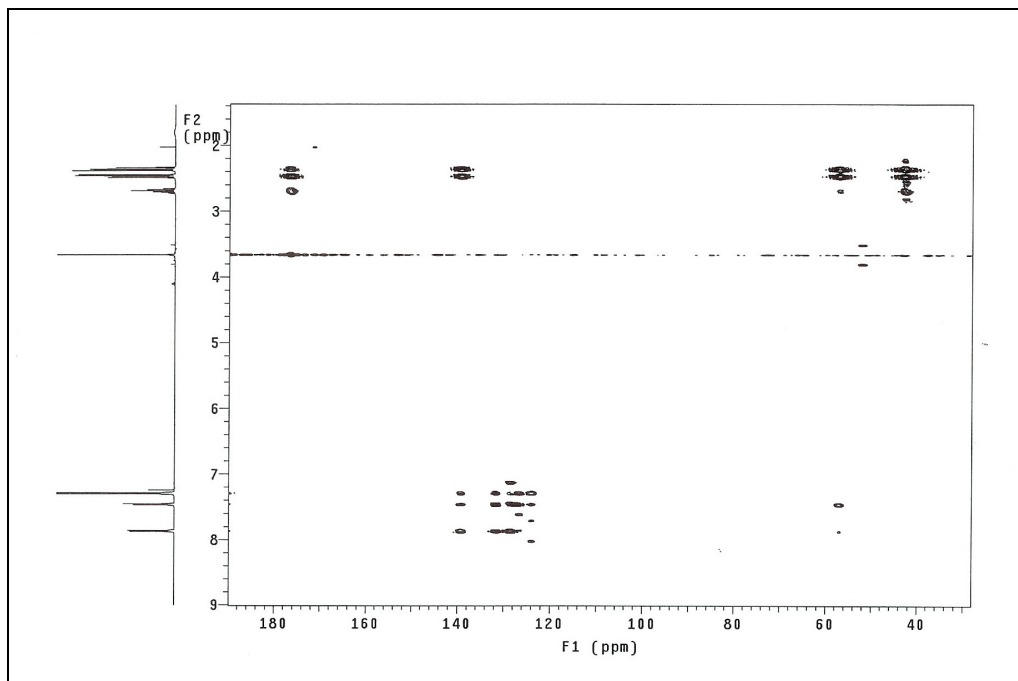
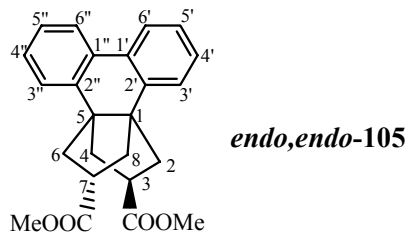


^{13}C -DEPT

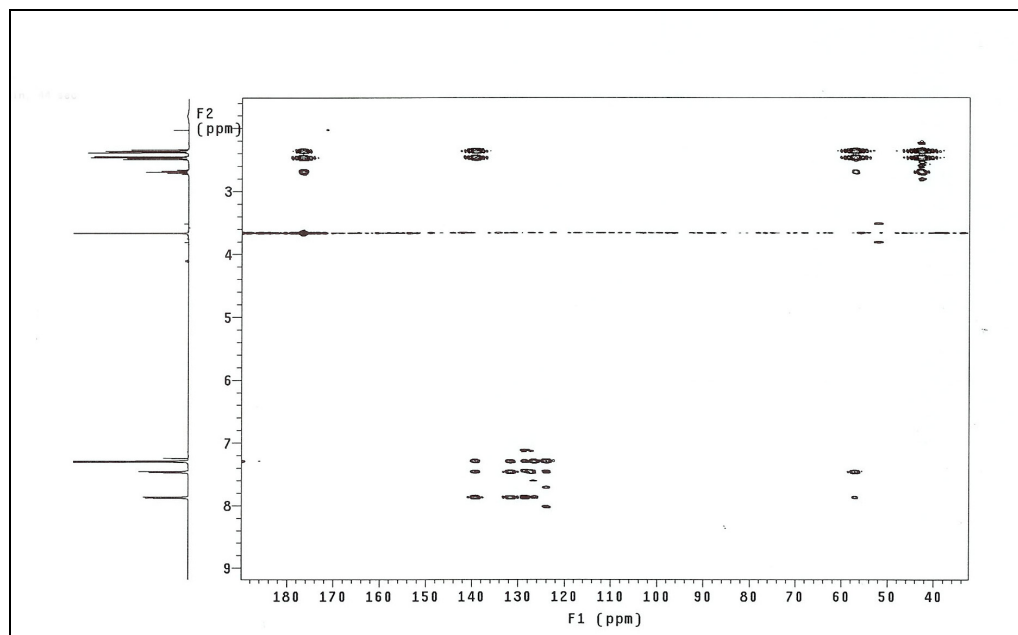


^1H - ^1H -COSY

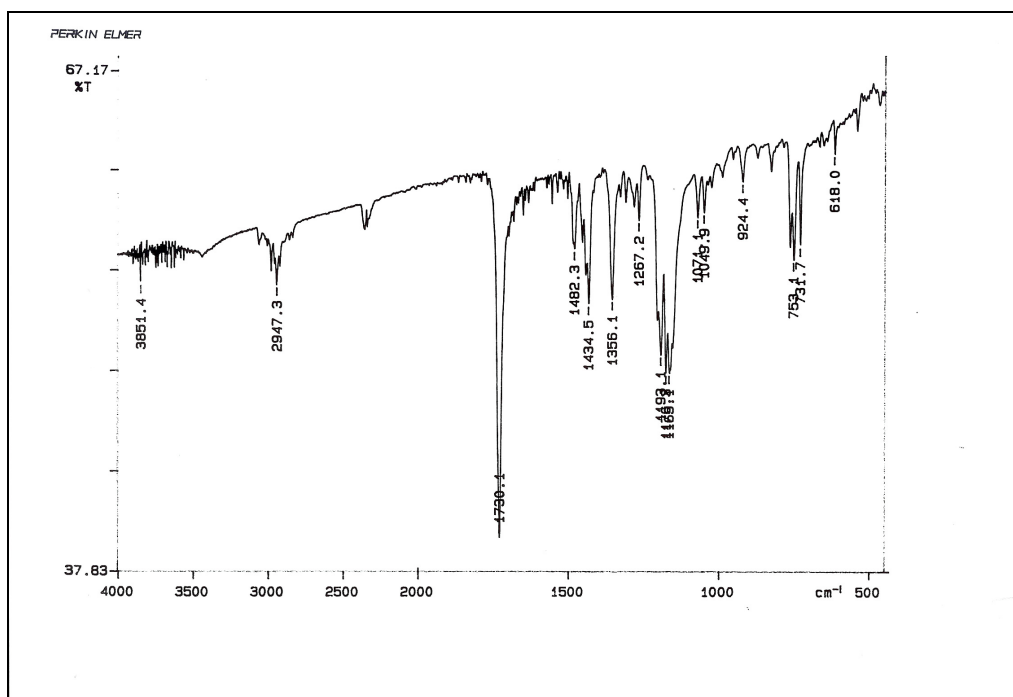
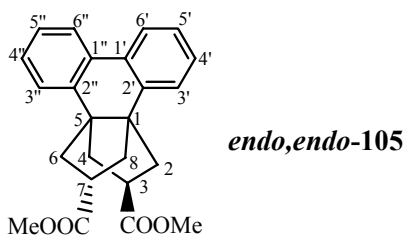
 ^1H - ^1H -NOESY ^1H - ^{13}C -HSQC



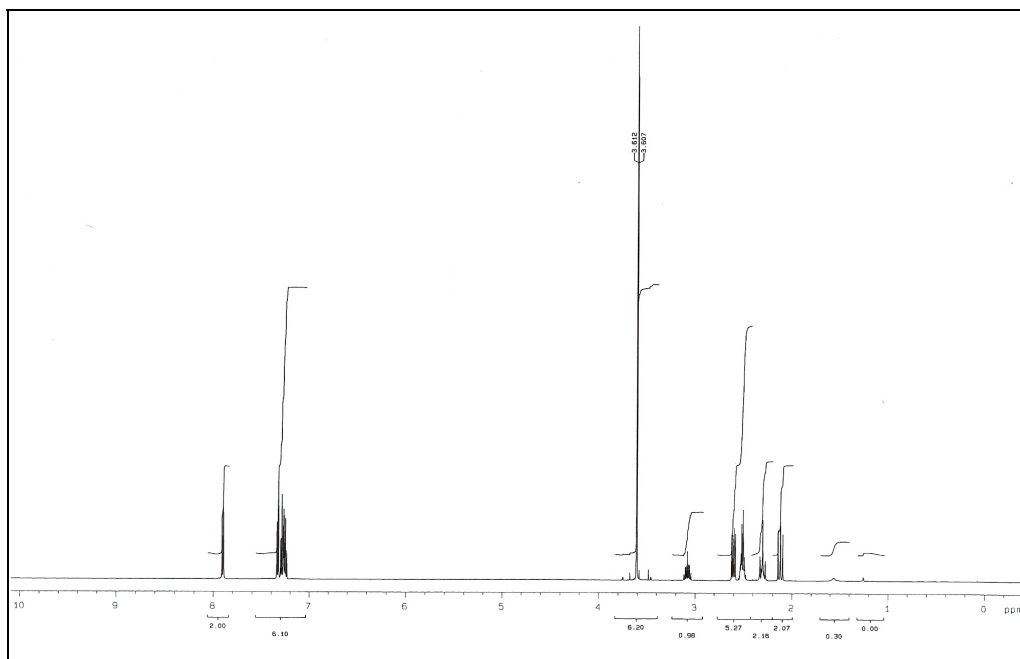
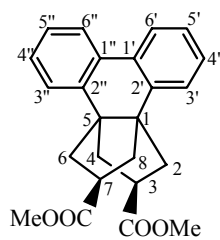
$^1\text{H}-^{13}\text{C}$ -HMBC $J = 8 \text{ Hz}$



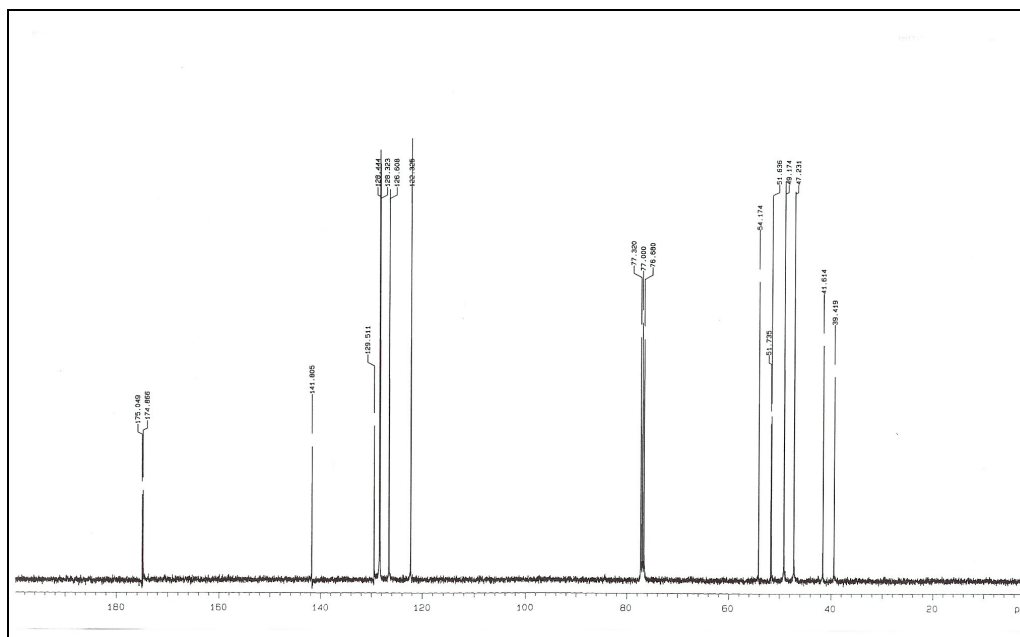
$^1\text{H}-^{13}\text{C}$ -HMBC $J = 5 \text{ Hz}$



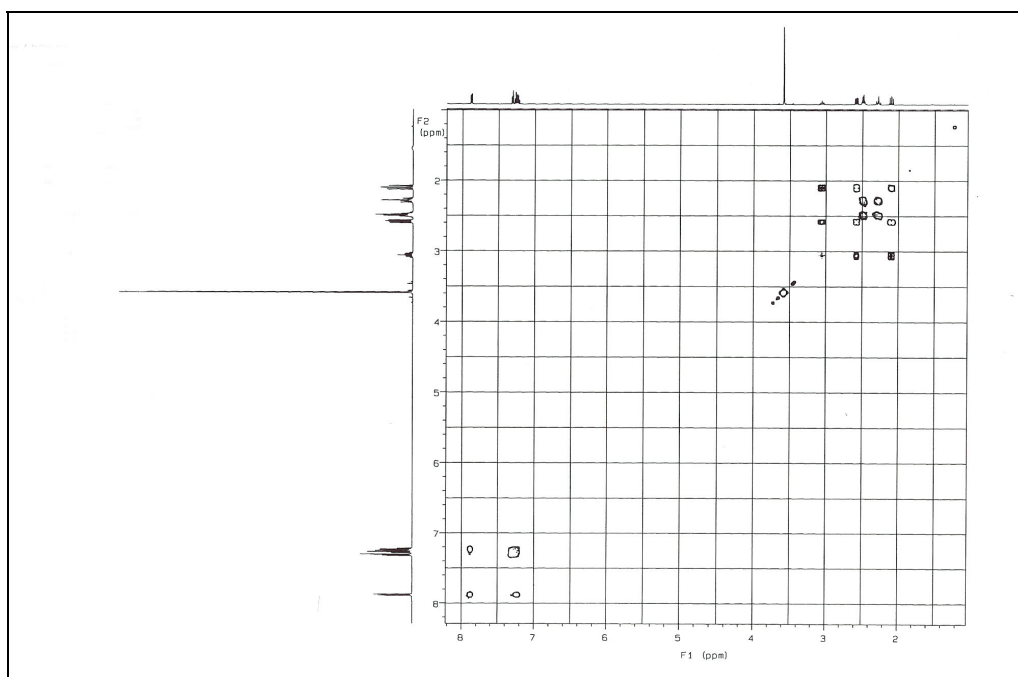
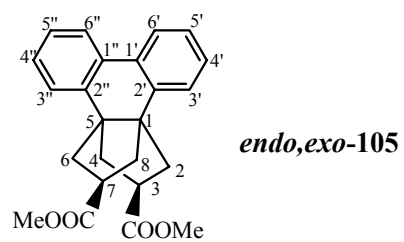
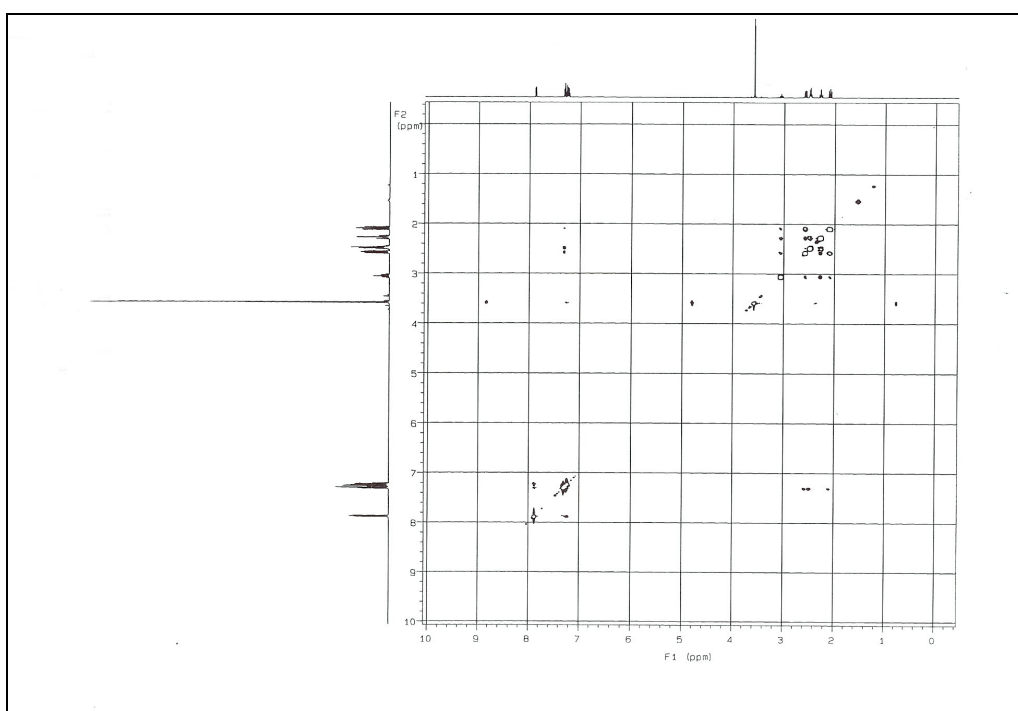
IR (KBr)

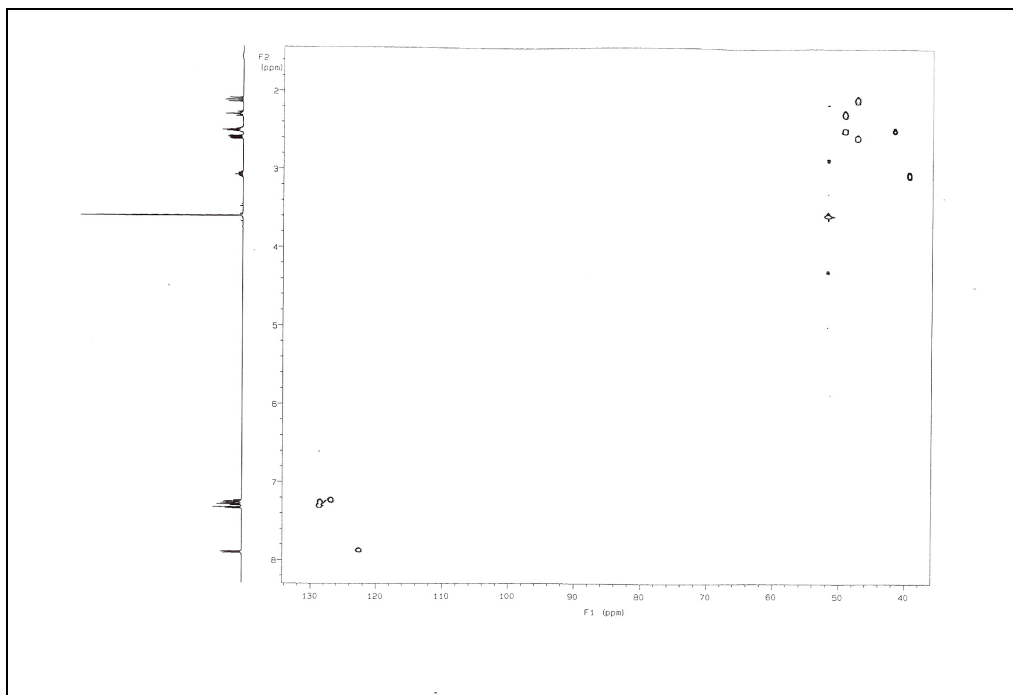
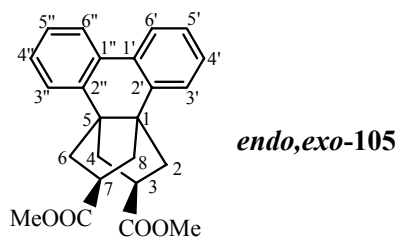


¹H-RMN (500 MHz, CDCl₃)

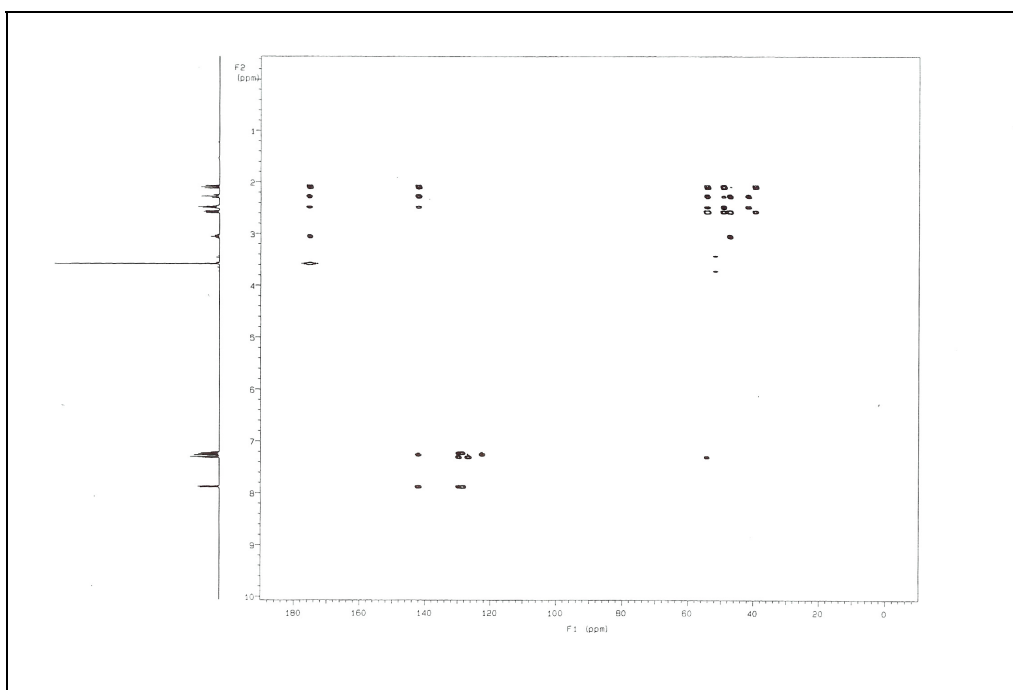


¹³C-RMN (100.6 MHz, CDCl₃)

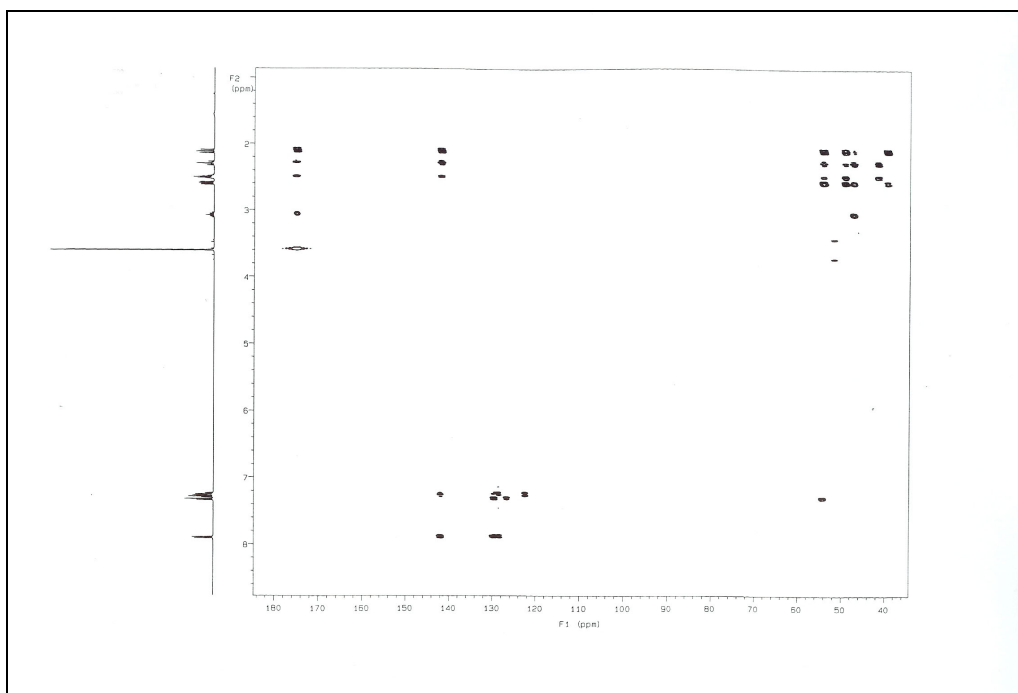
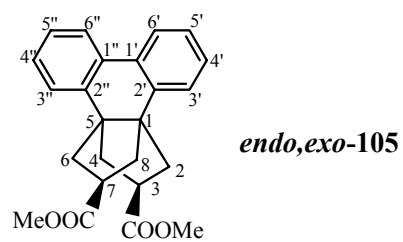
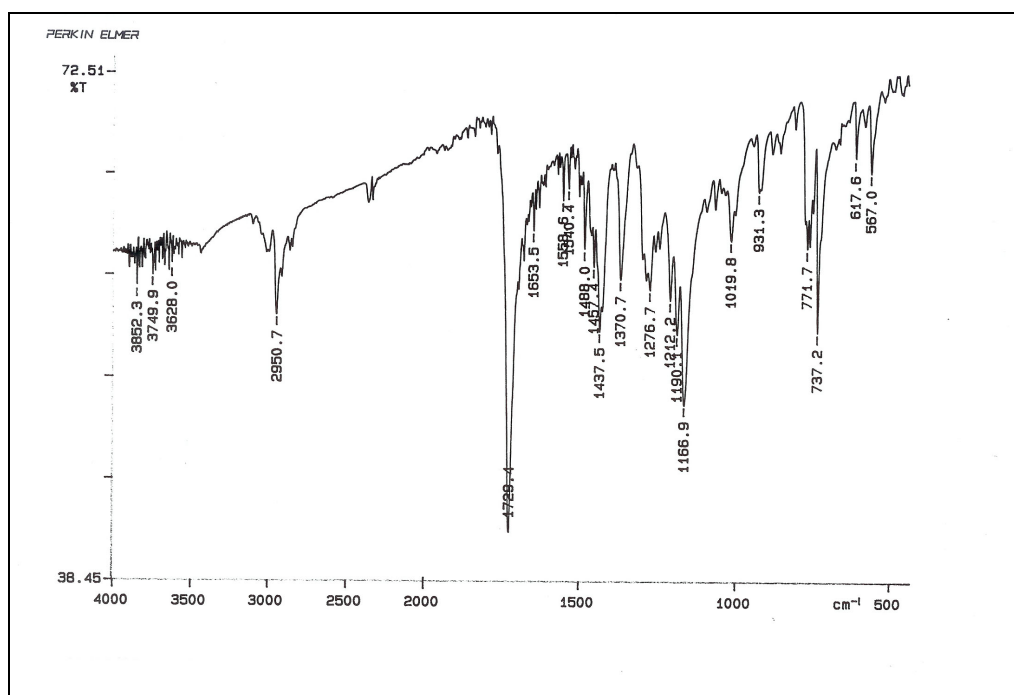
 ^1H - ^1H -COSY ^1H - ^1H -NOESY



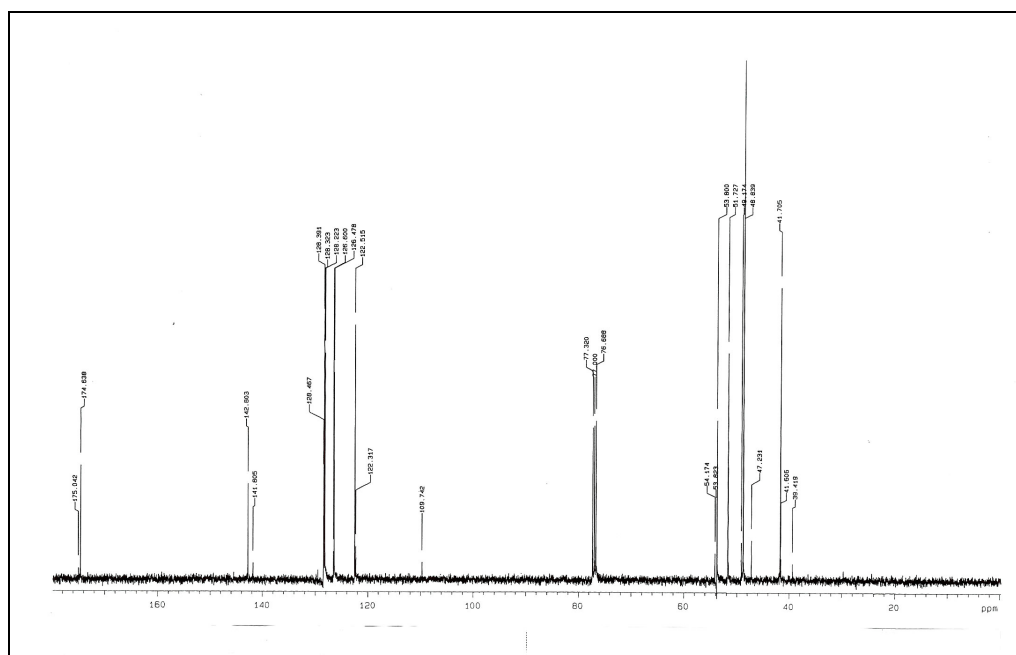
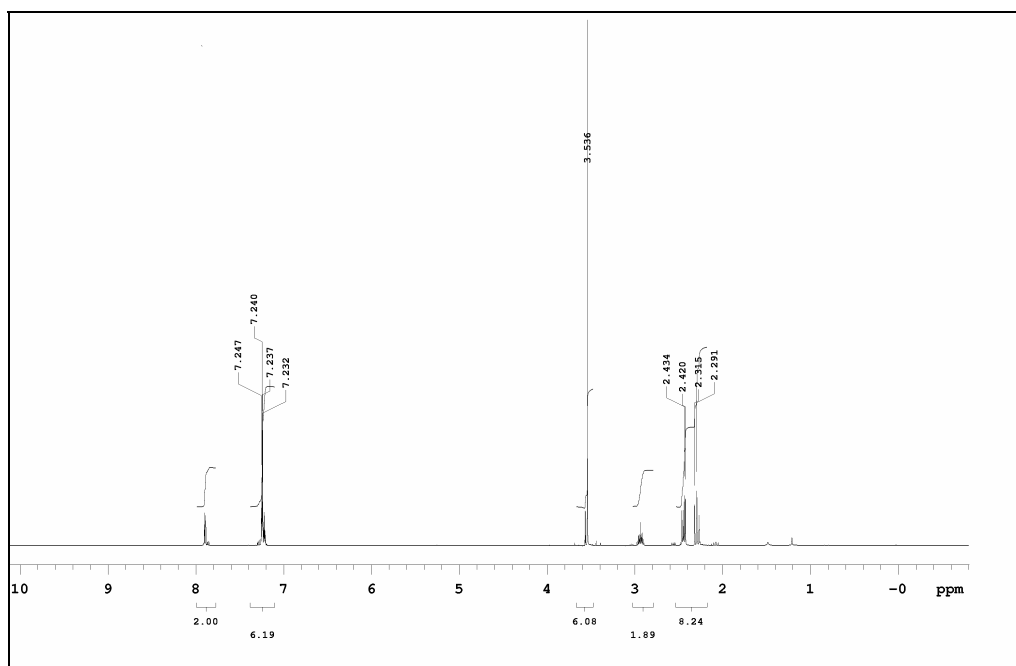
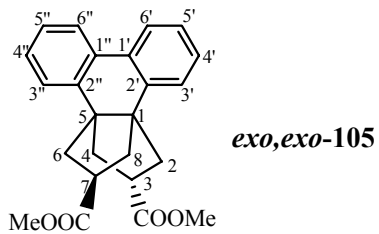
$^1\text{H}-^{13}\text{C}\text{-HSQC}$

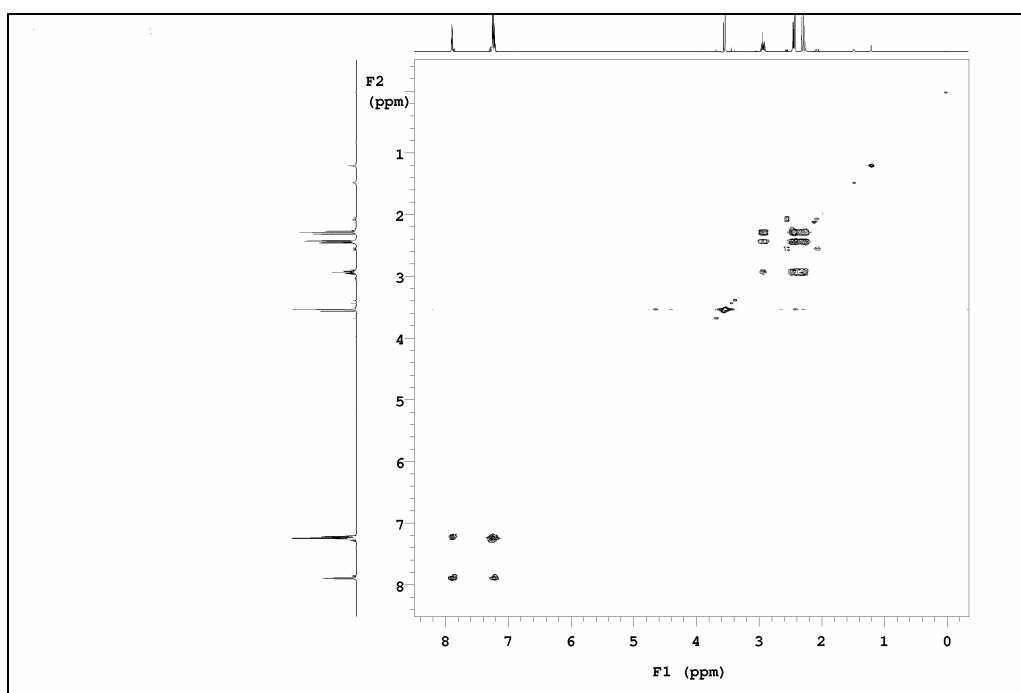
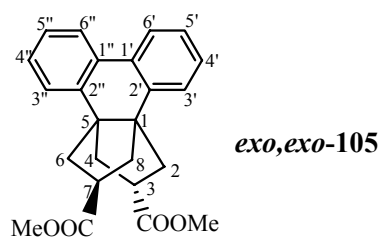
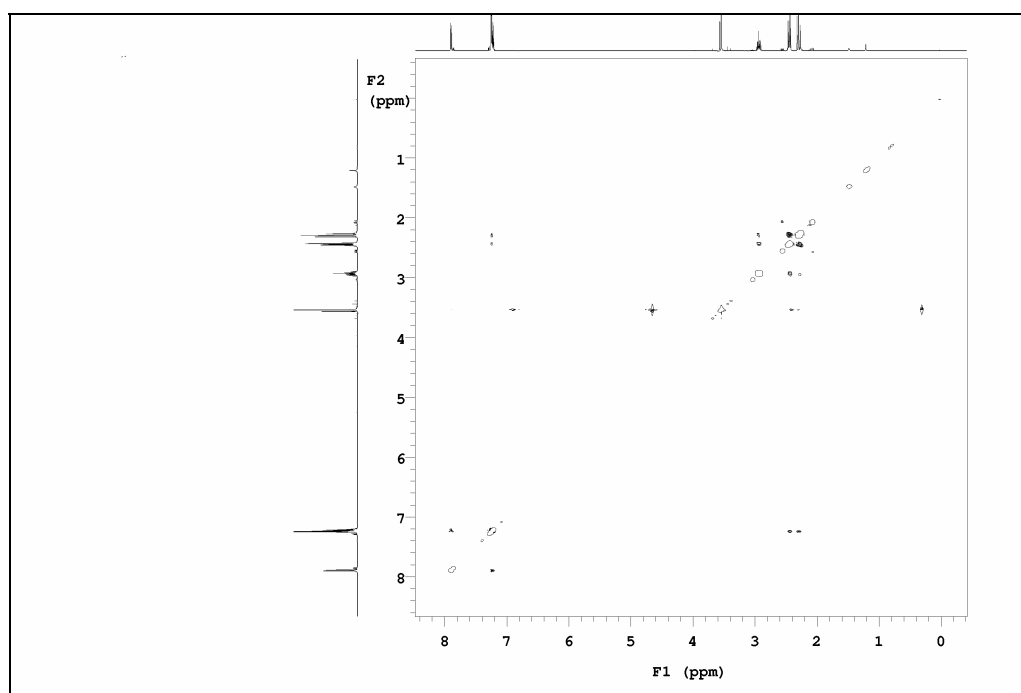


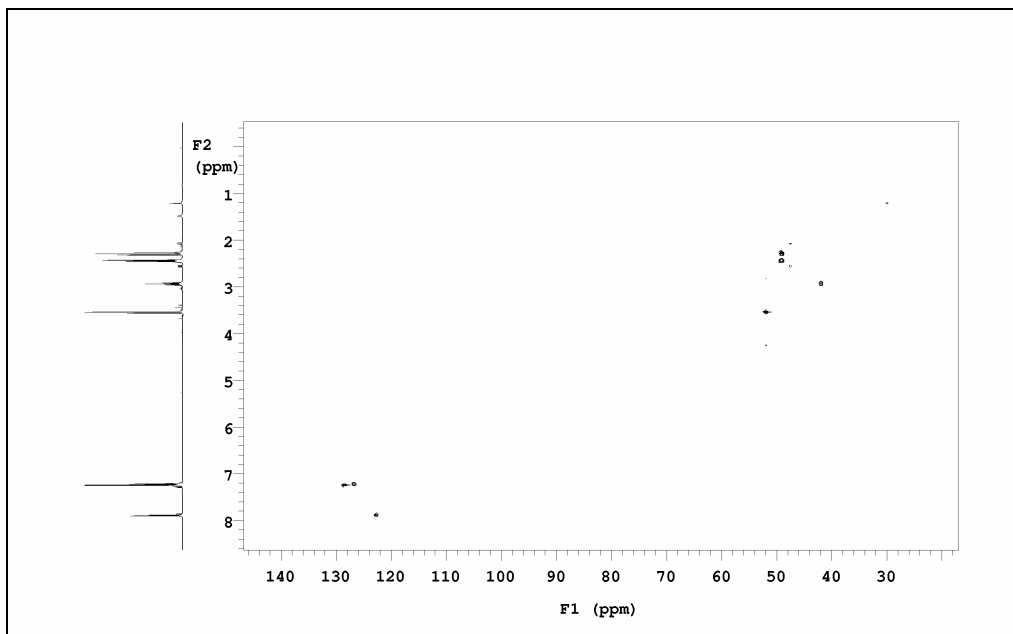
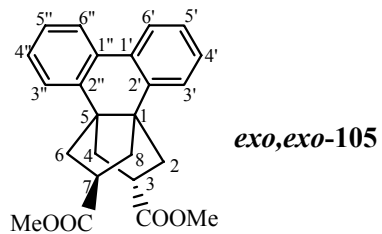
$^1\text{H}-^{13}\text{C}\text{-HMBC } J = 8 \text{ Hz}$


 $^1\text{H}-^{13}\text{C}\text{-HMBC } J = 5 \text{ Hz}$


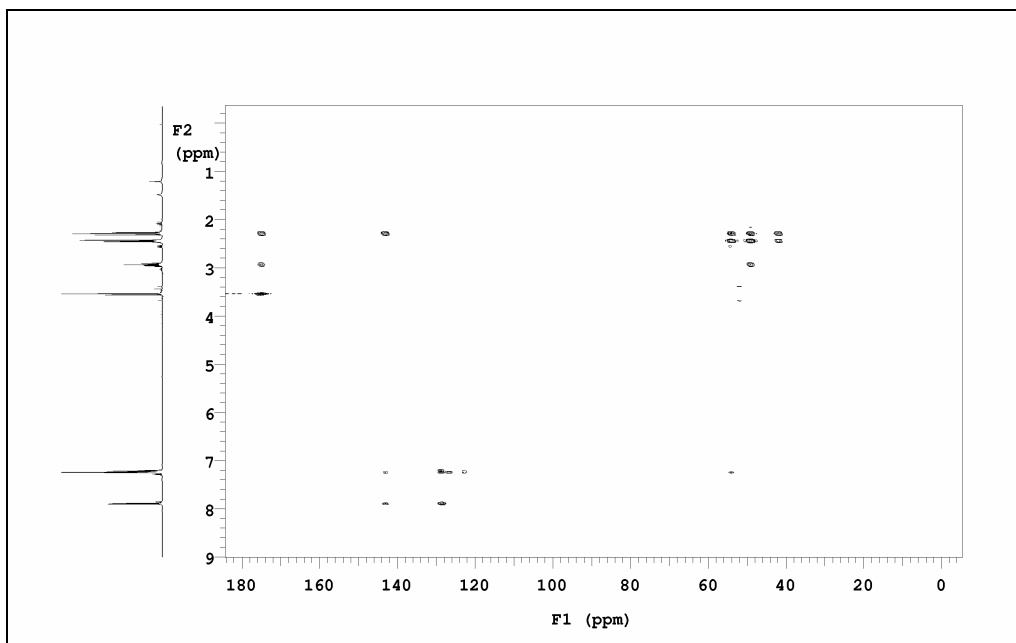
IR (KBr)



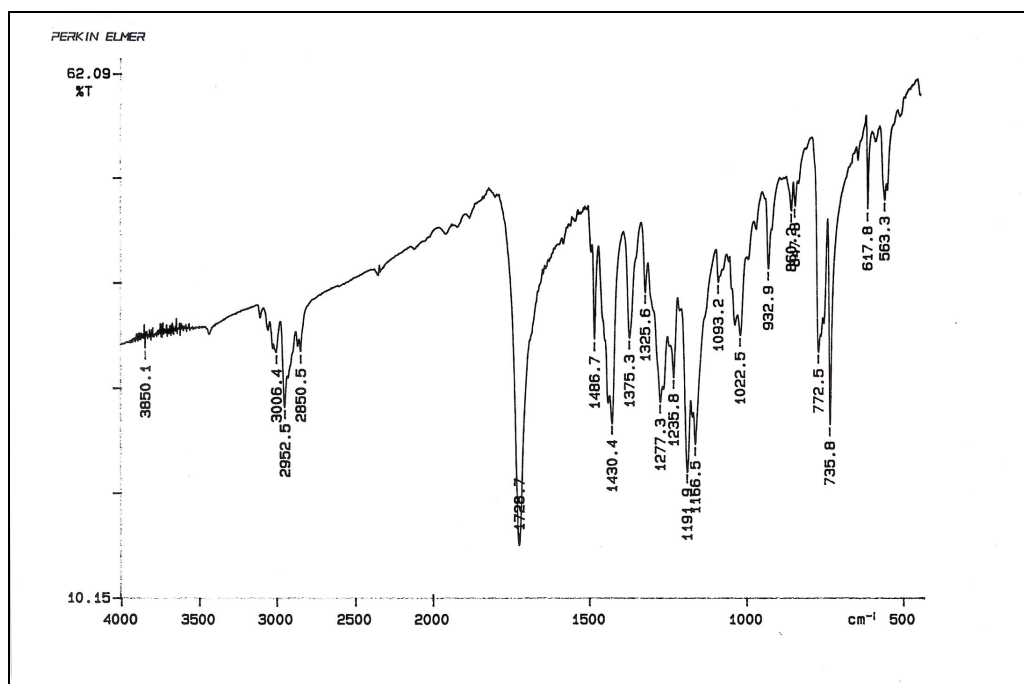
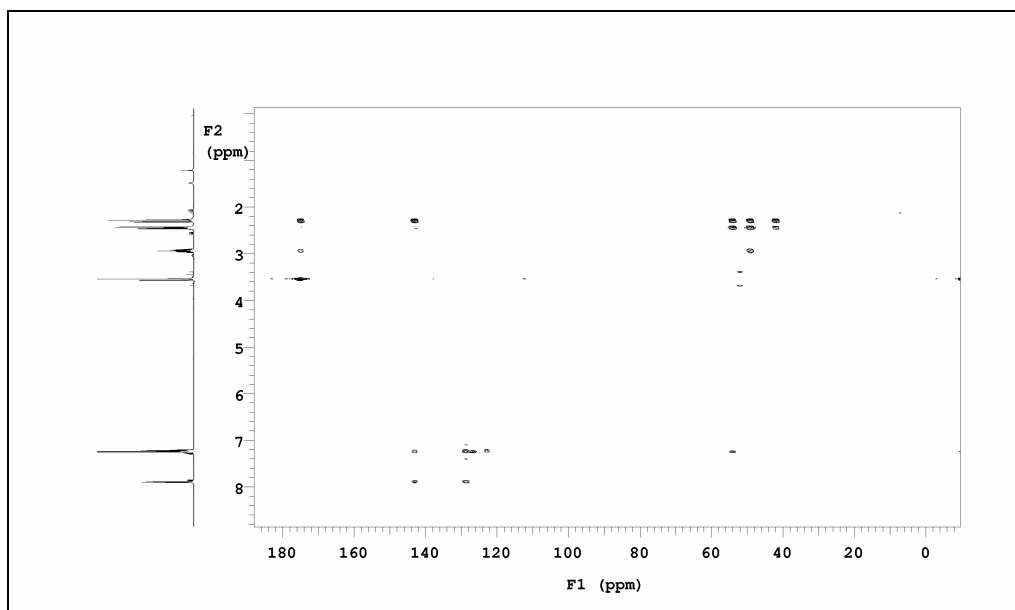
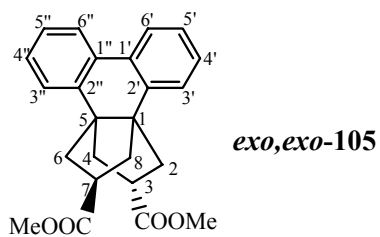
 ^1H - ^1H -COSY ^1H - ^1H -NOESY



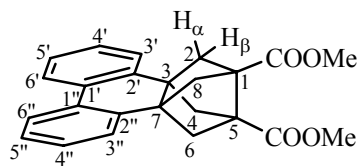
$^1\text{H}-^{13}\text{C}$ -HSQC



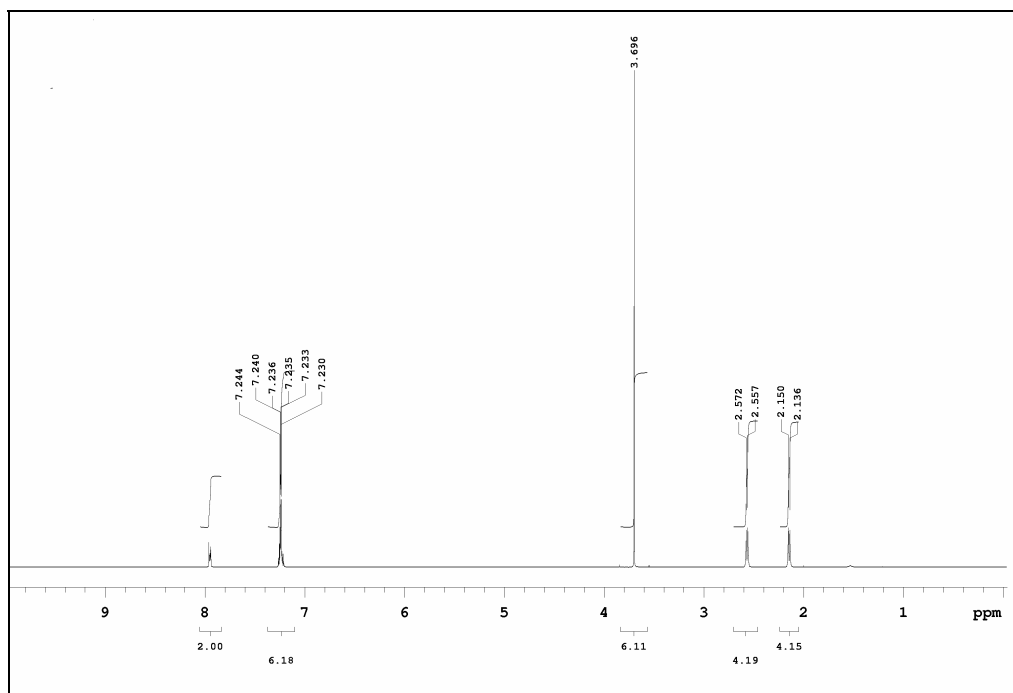
$^1\text{H}-^{13}\text{C}$ -HMBC $J = 8 \text{ Hz}$



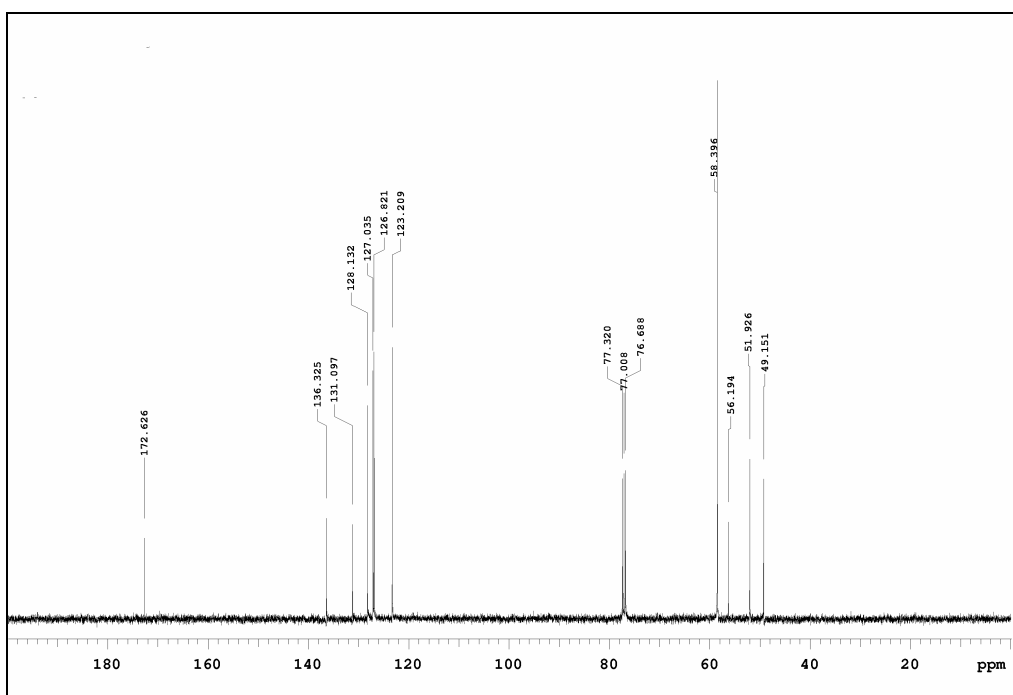
IR (KBr)



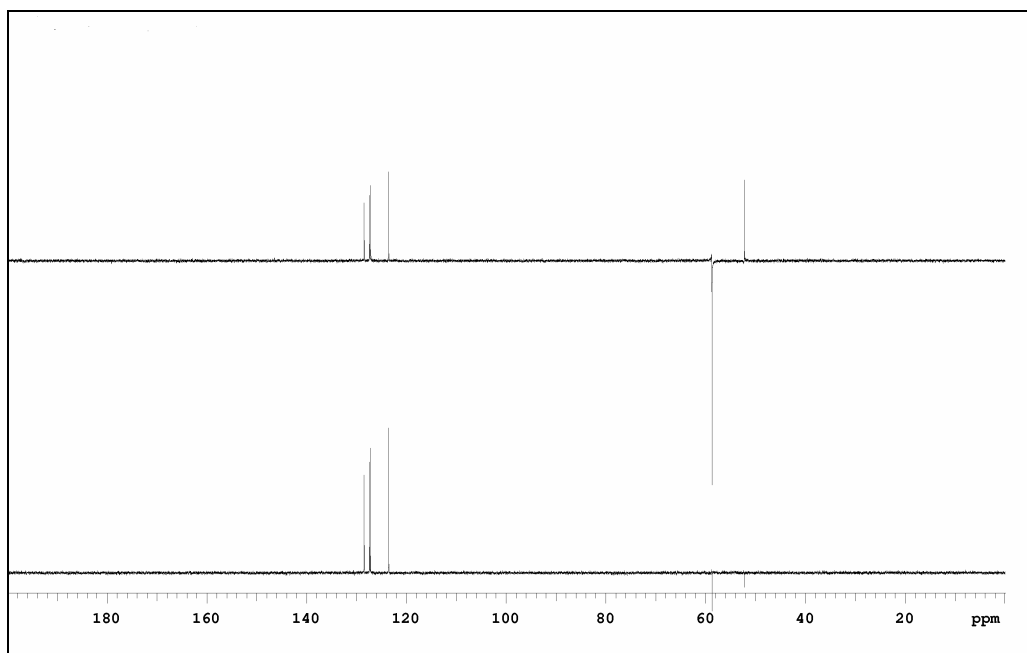
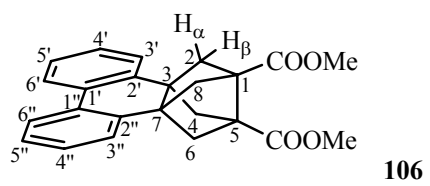
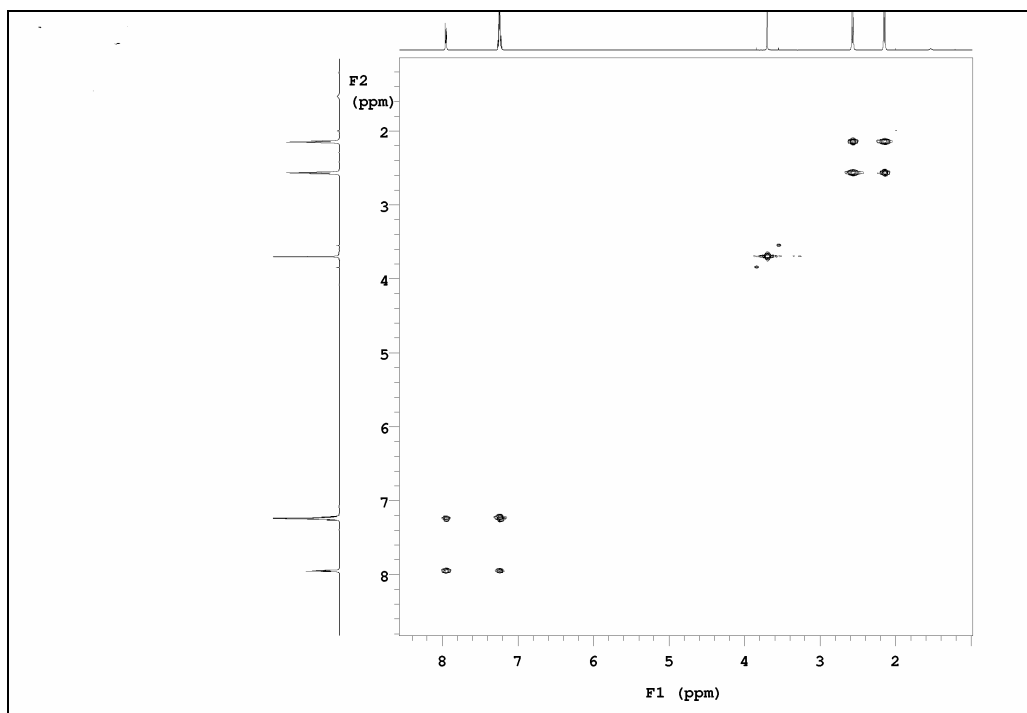
106

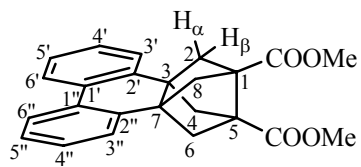


$^1\text{H-RMN}$ (500 MHz, CDCl_3)

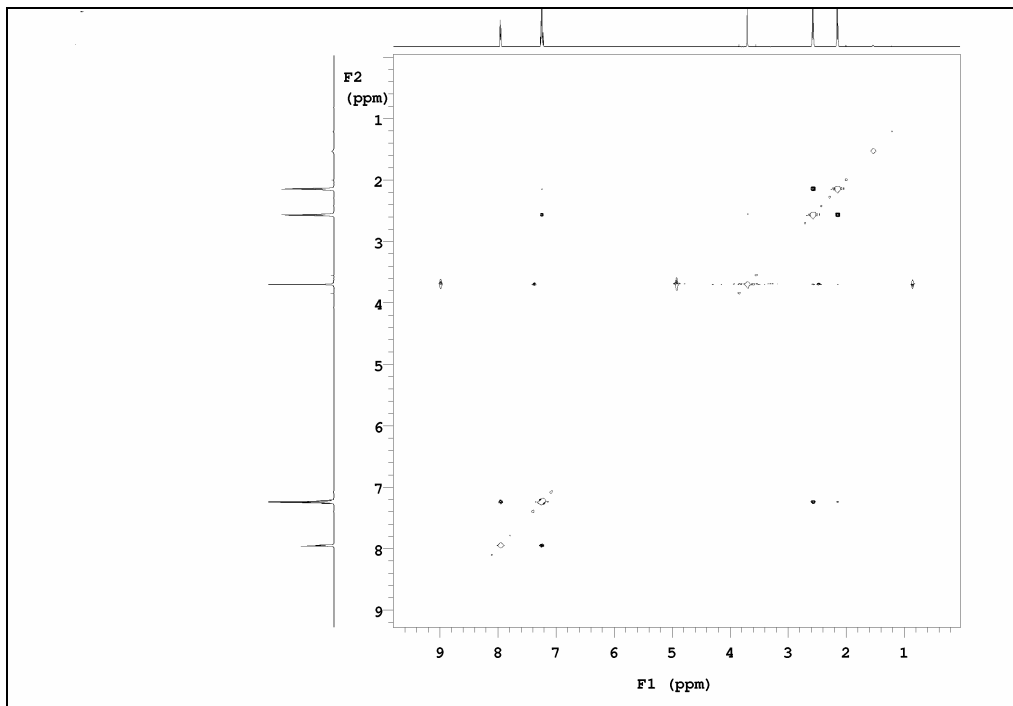


$^{13}\text{C-RMN}$ (100.6 MHz, CDCl_3)

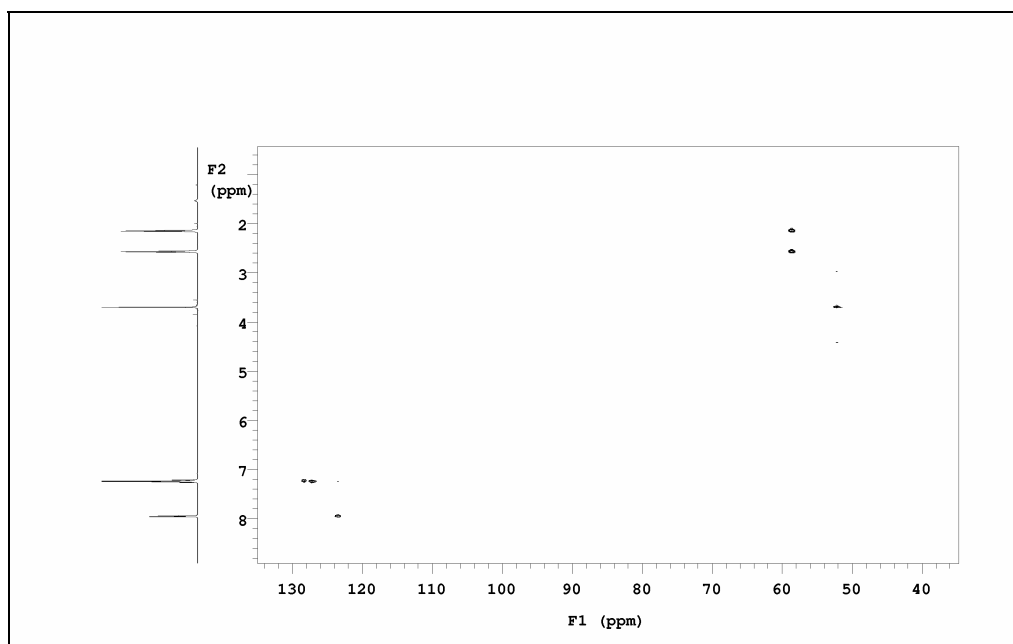
 ^{13}C -DEPT ^1H - ^1H -COSY



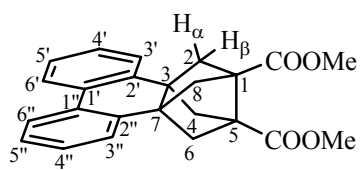
106



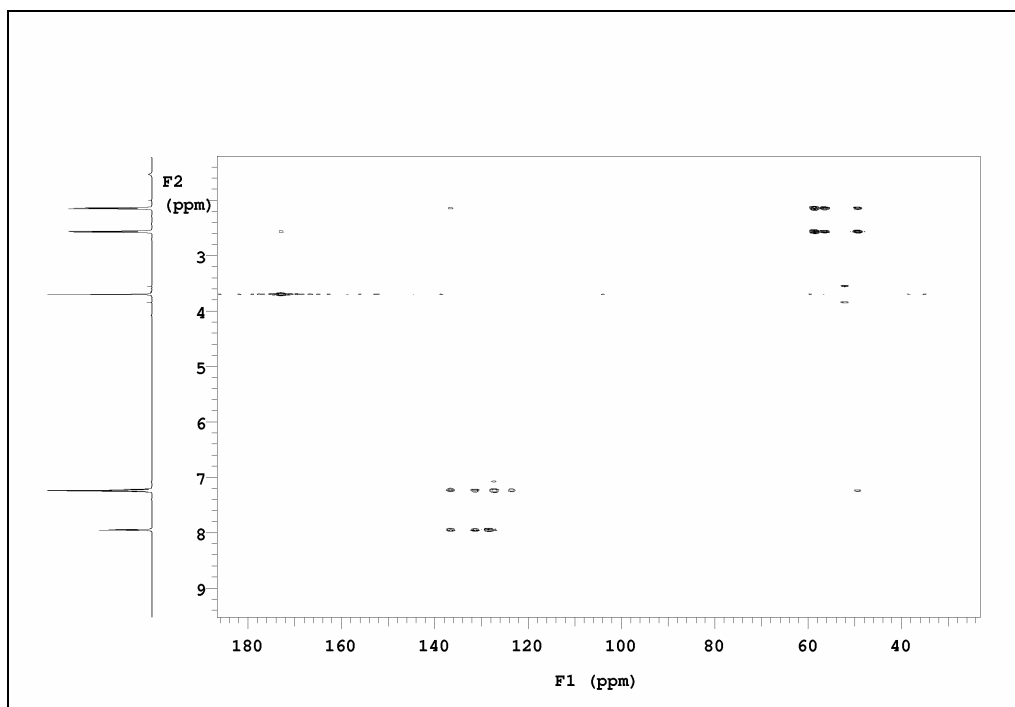
^1H - ^1H -NOESY



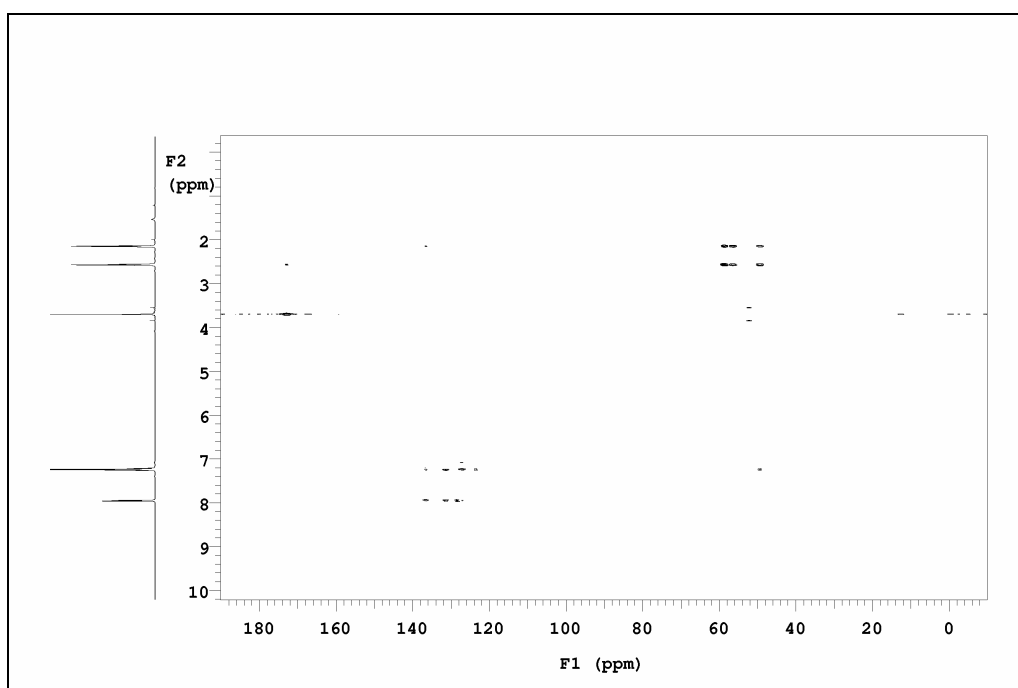
^1H - ^{13}C -HSQC



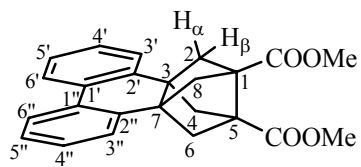
106



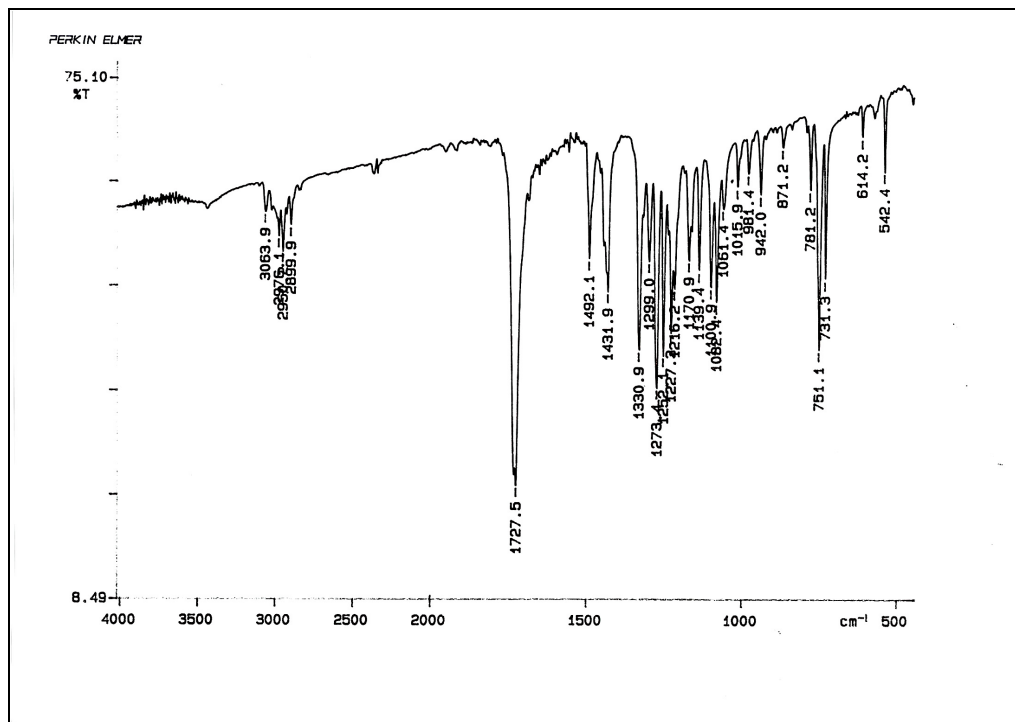
$^1\text{H}-^{13}\text{C}$ -HMBC $J = 8 \text{ Hz}$



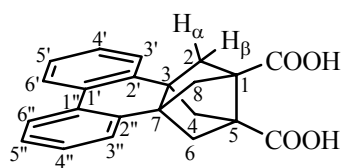
$^1\text{H}-^{13}\text{C}$ -HMBC $J = 5 \text{ Hz}$



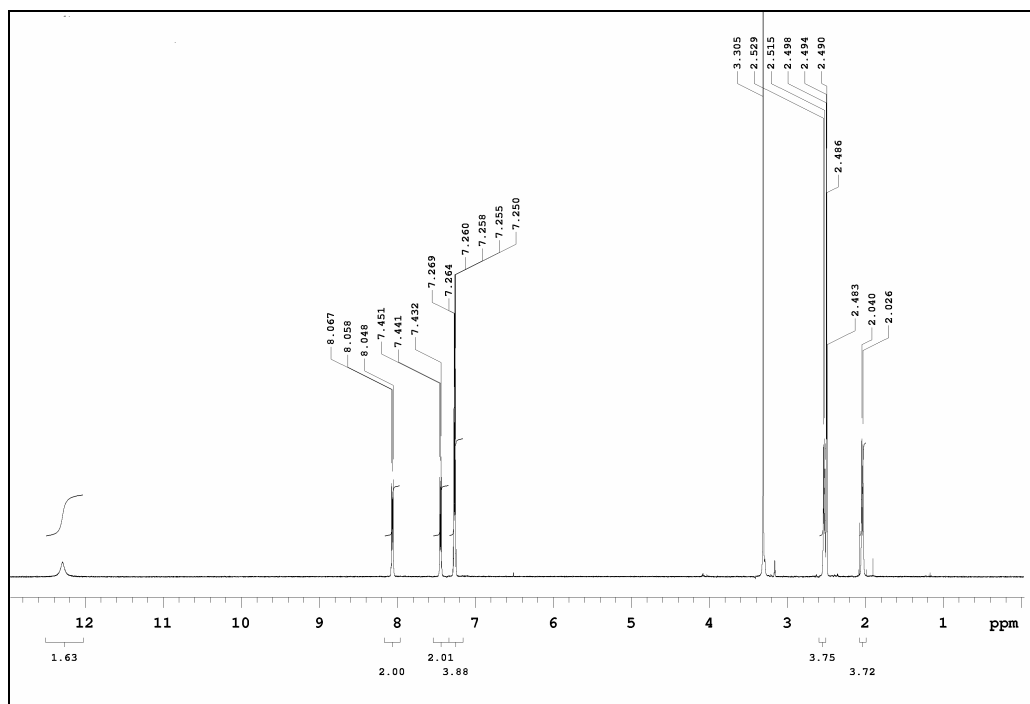
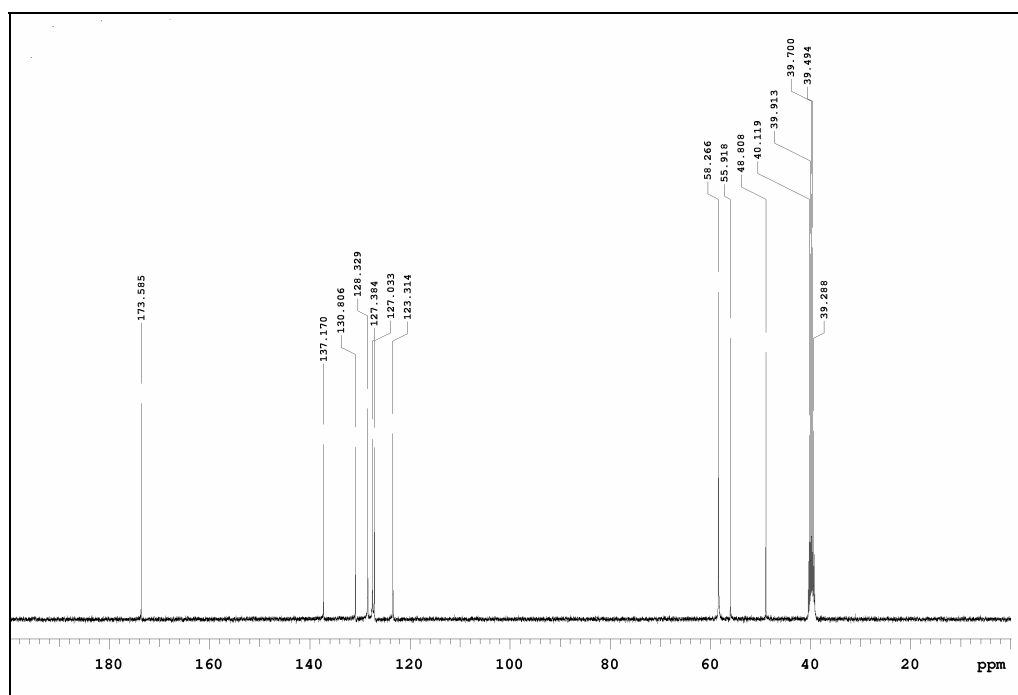
106

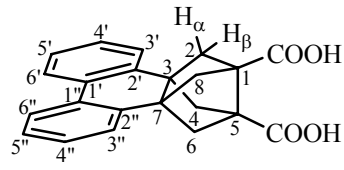


IR (KBr)

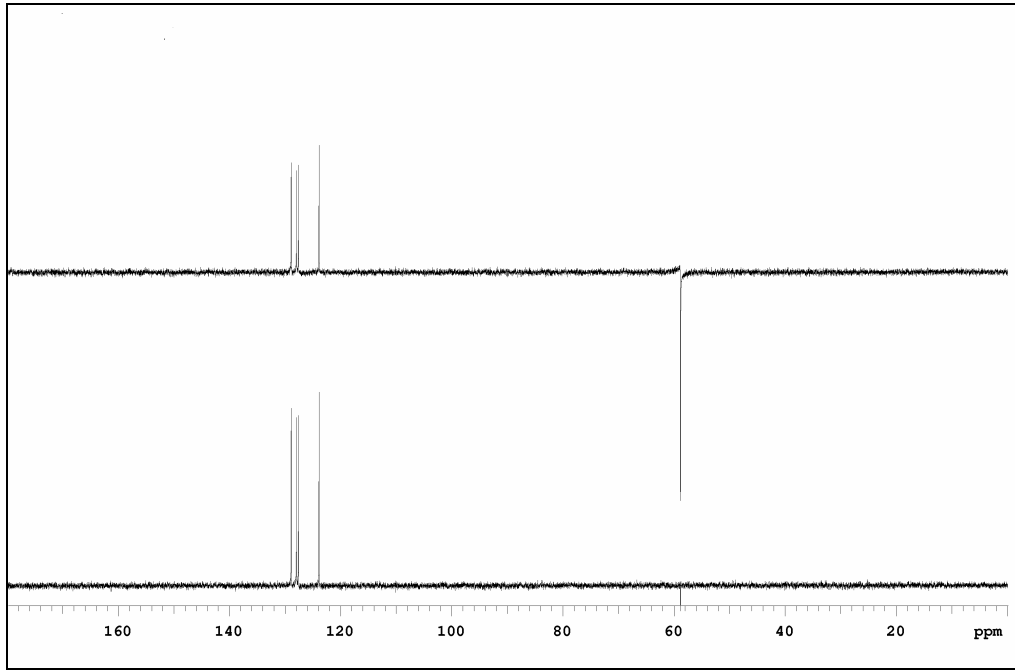


120

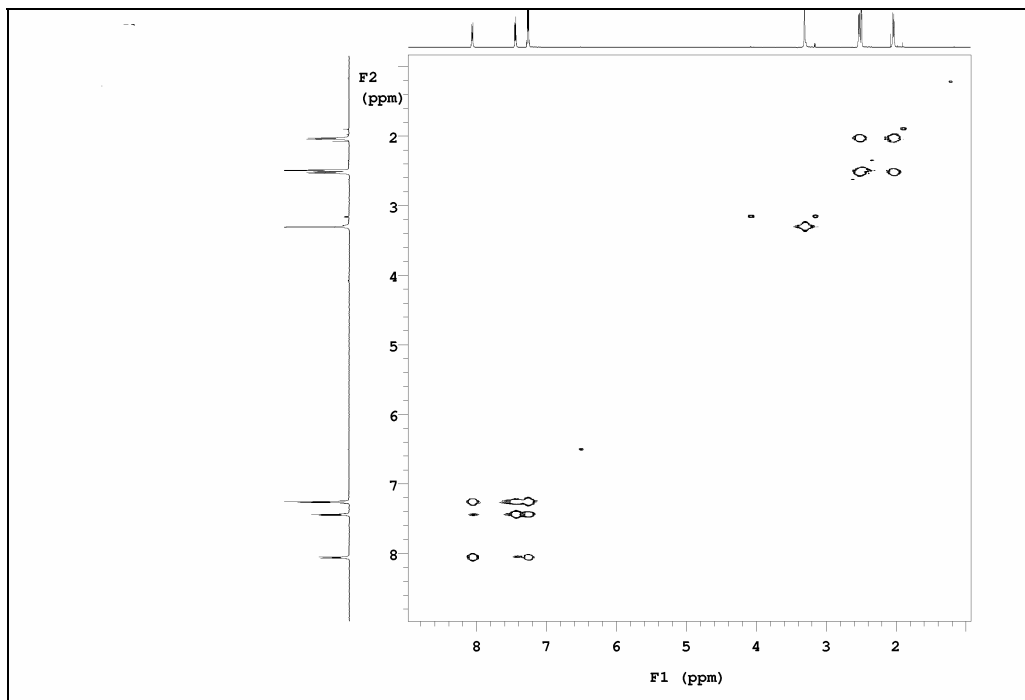
 ^1H -RMN (500 MHz, DMSO-d_6) ^{13}C -RMN (100.6 MHz, DMSO-d_6)



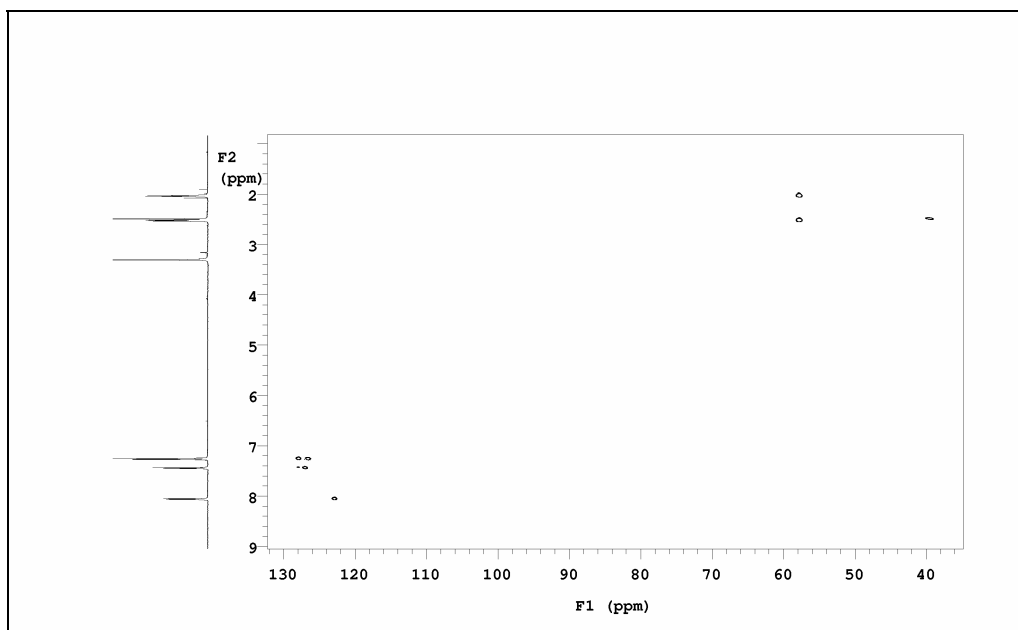
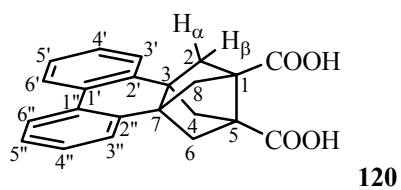
120



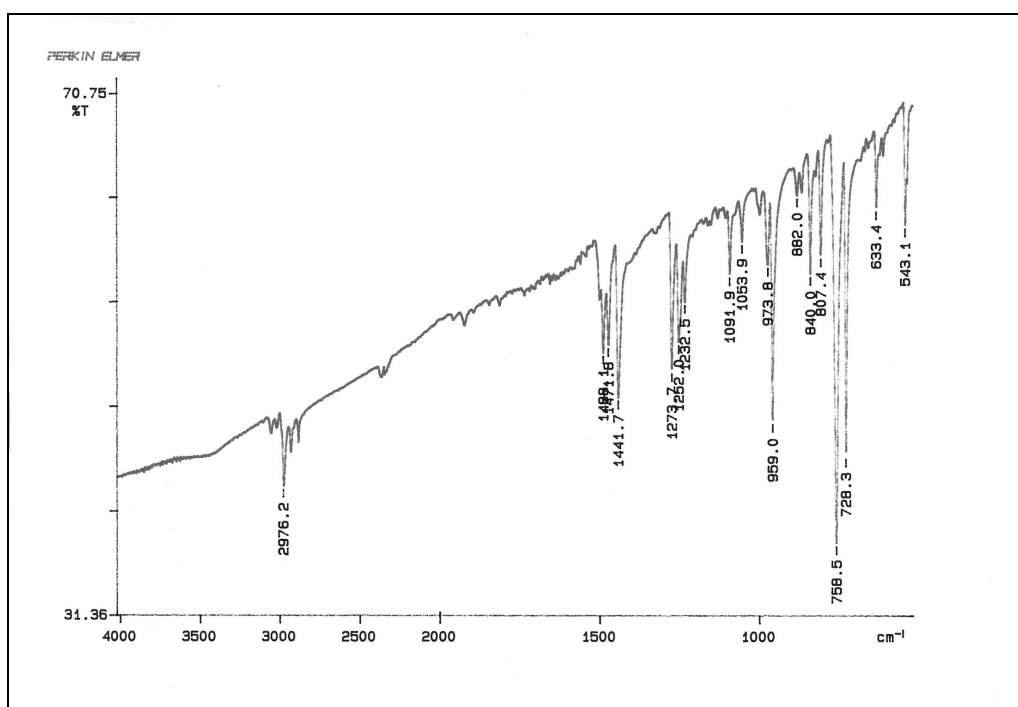
¹³C-DEPT



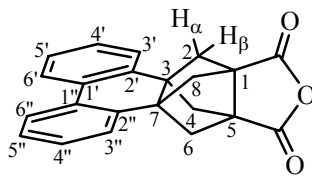
¹H-¹H-COSY



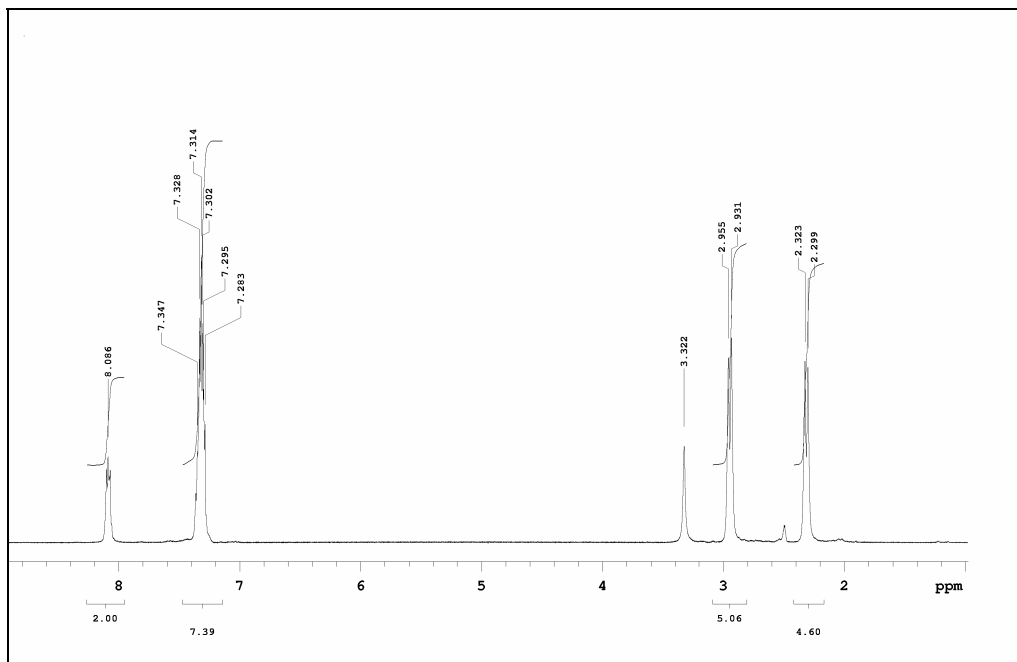
$^1\text{H}-^{13}\text{C}\text{-HSQC}$



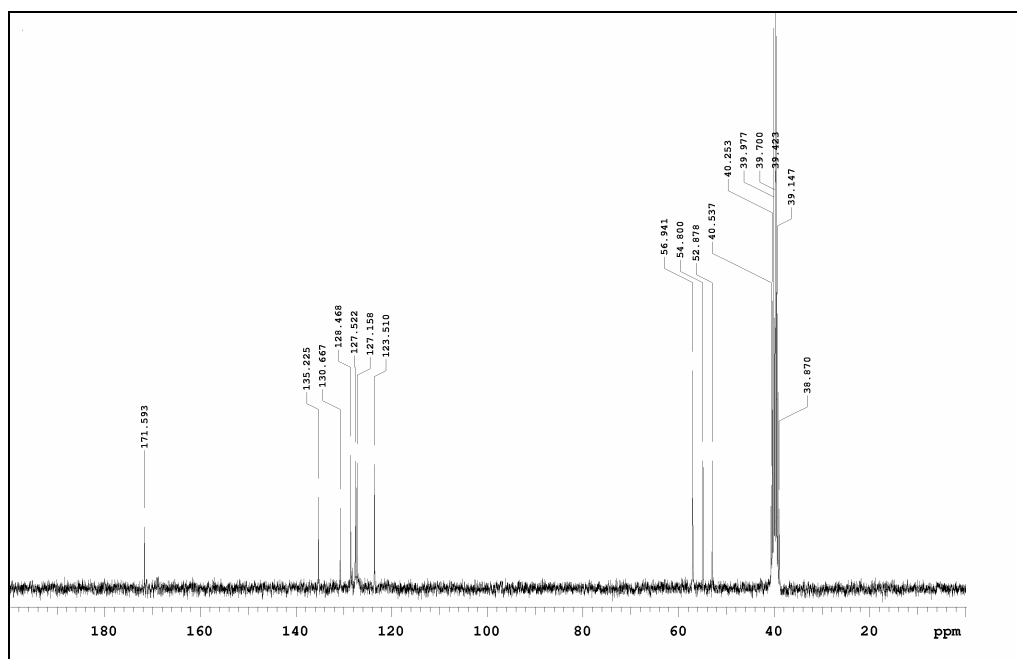
IR (KBr)



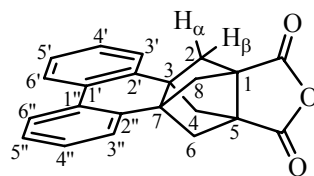
121



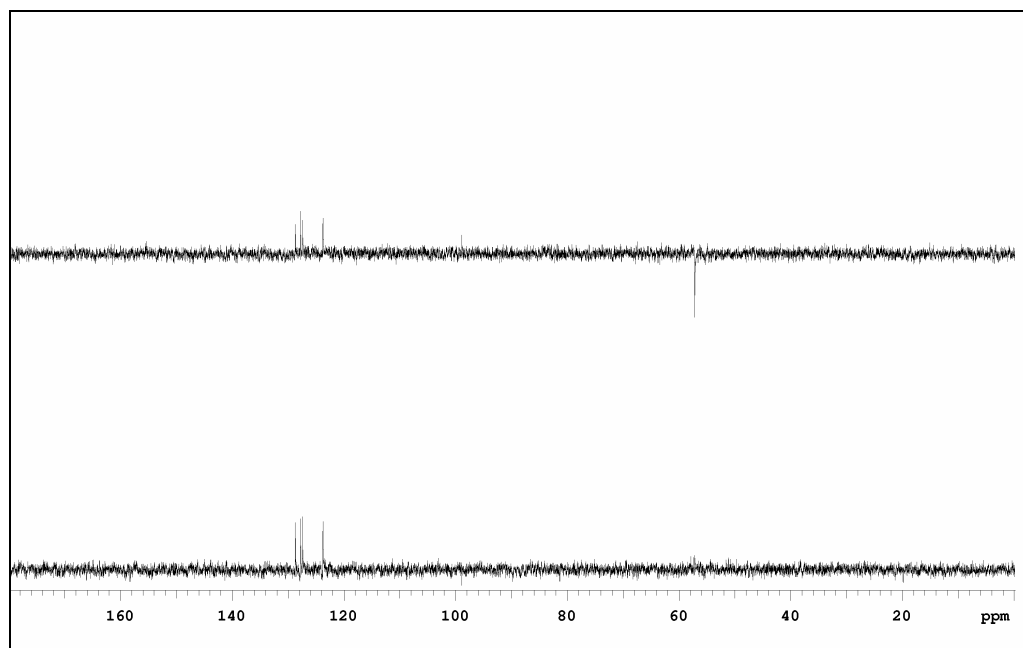
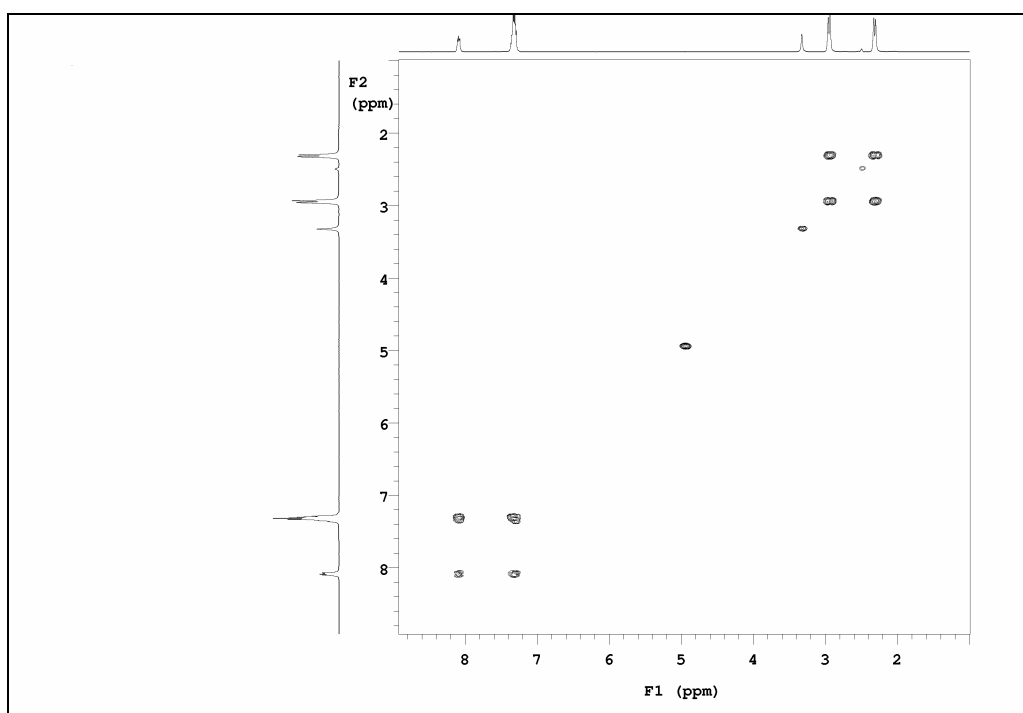
^1H -RMN (300 MHz, DMSO- d_6)

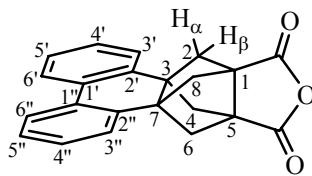


^{13}C -RMN (75.4 MHz, DMSO- d_6)

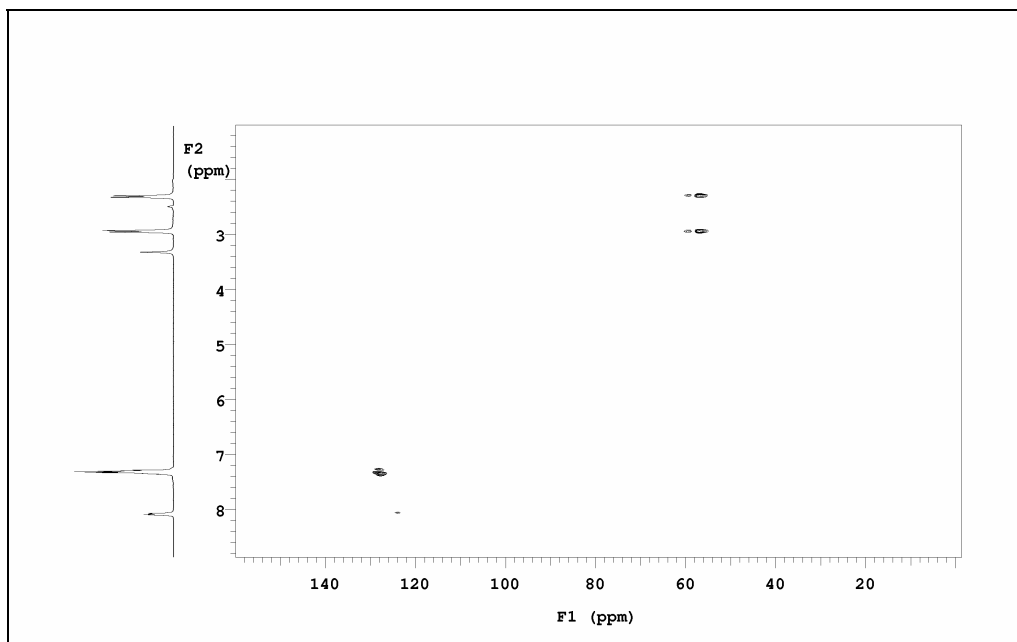


121

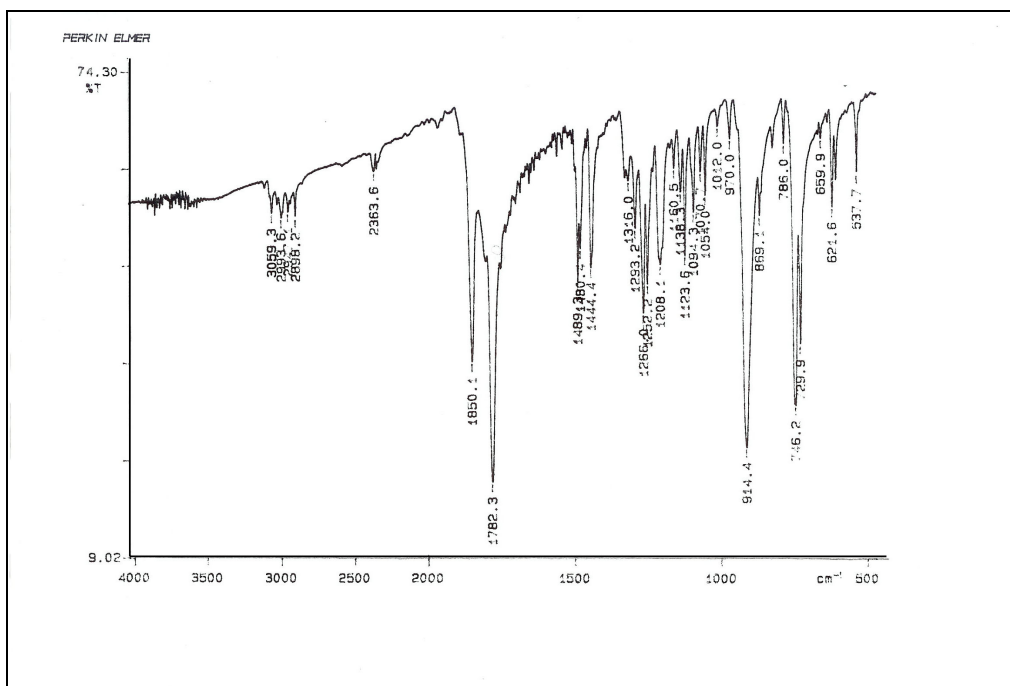
 $^{13}\text{C-DEPT}$  $^1\text{H-}^1\text{H-COSY}$



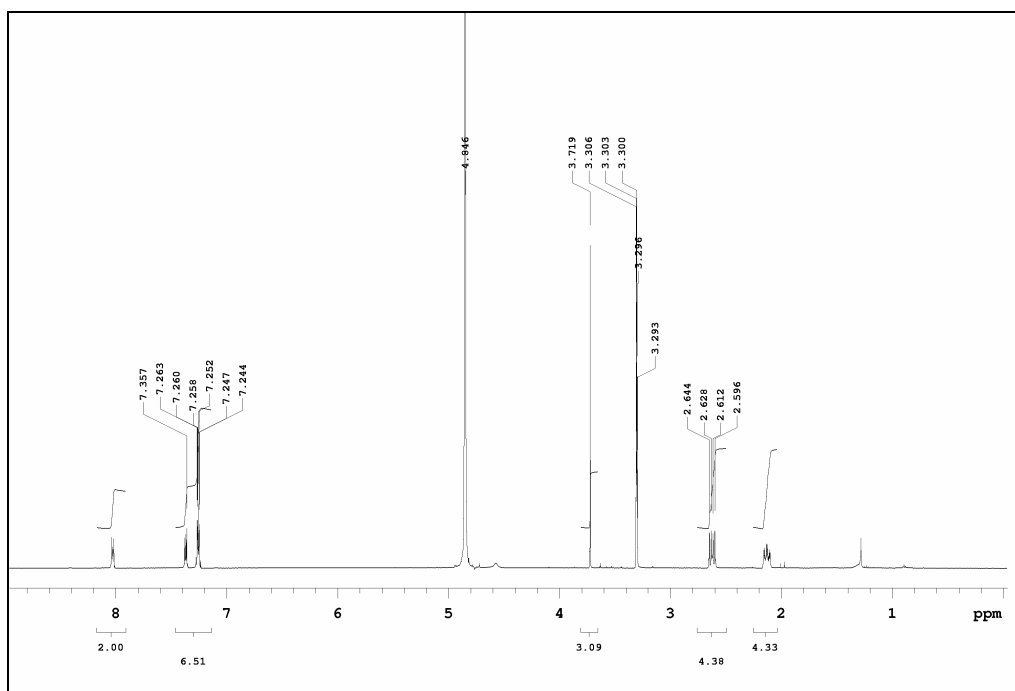
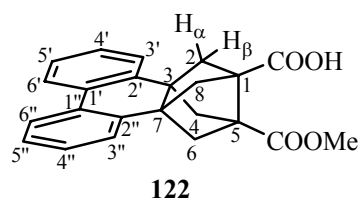
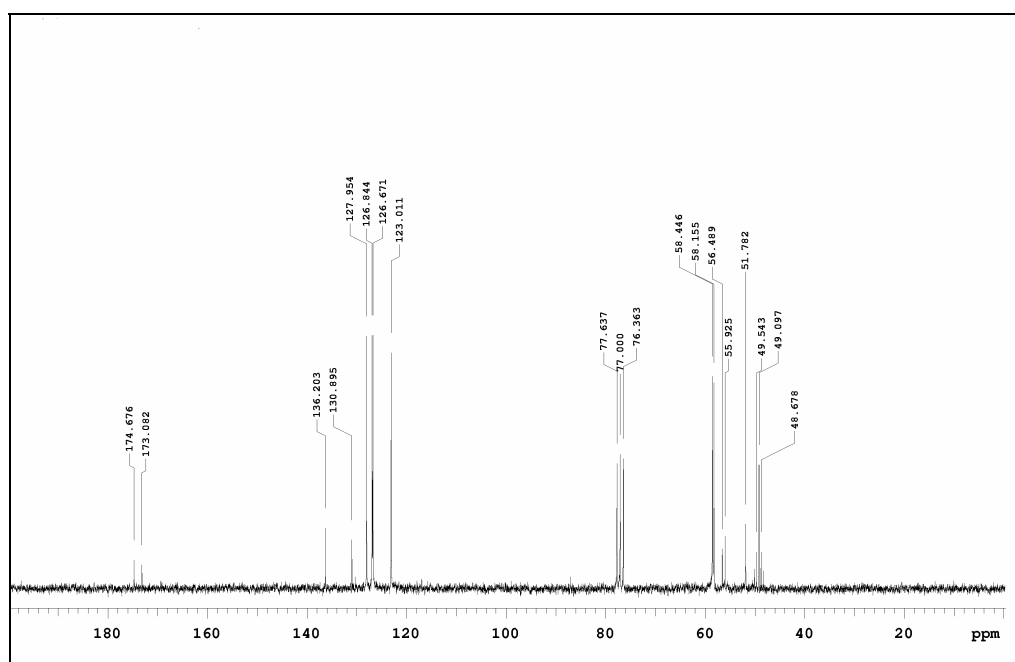
121

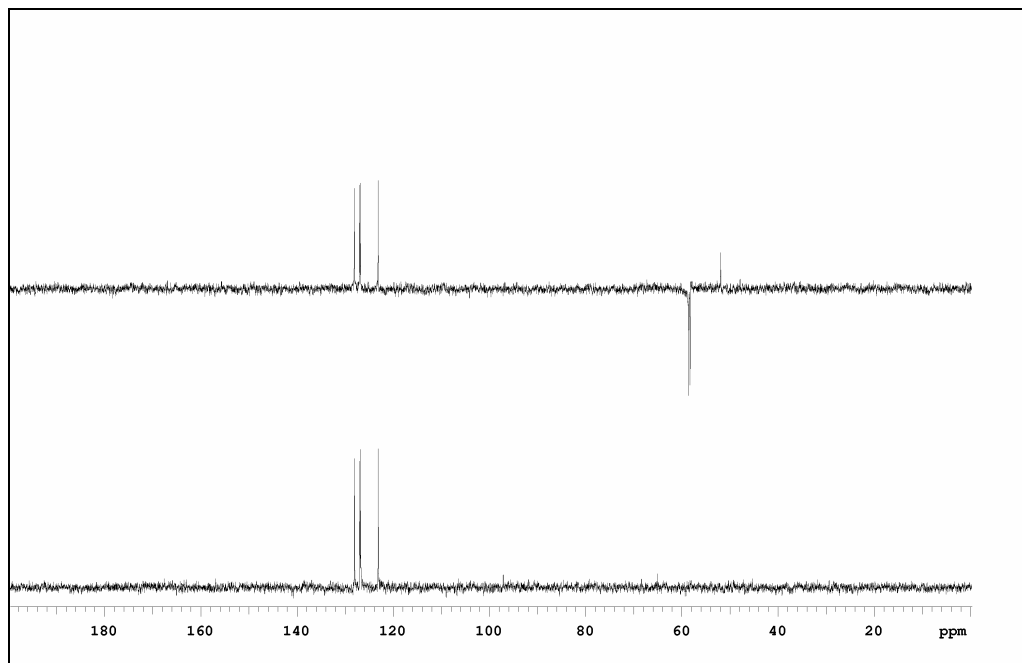
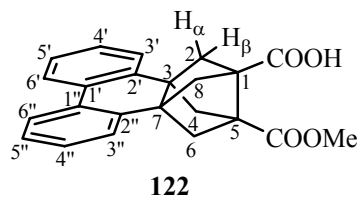


¹H-¹³C-HSQC

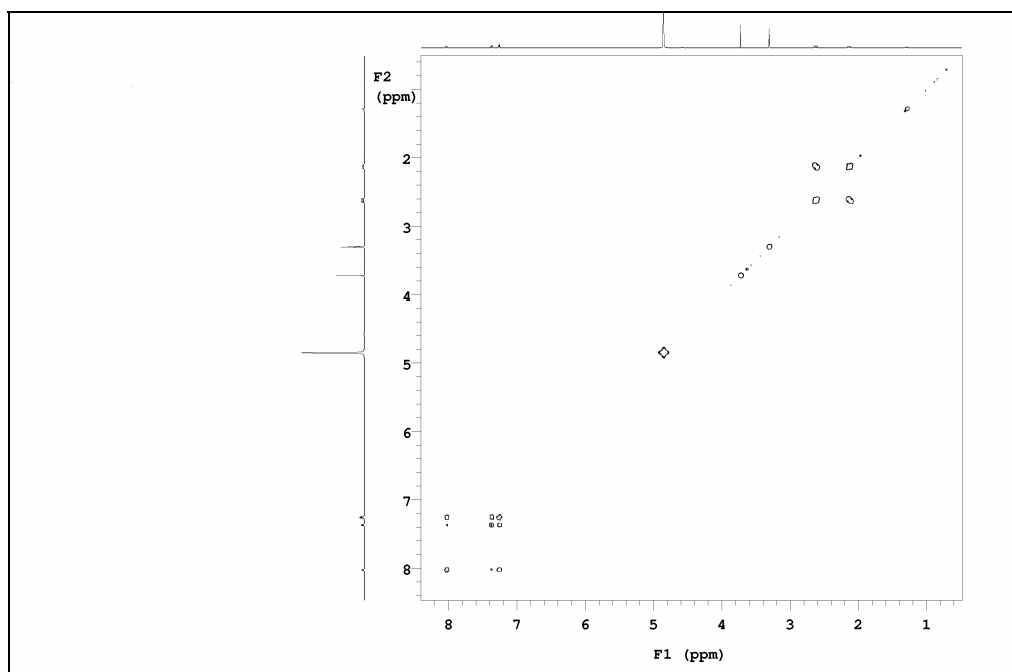


IR (KBr)

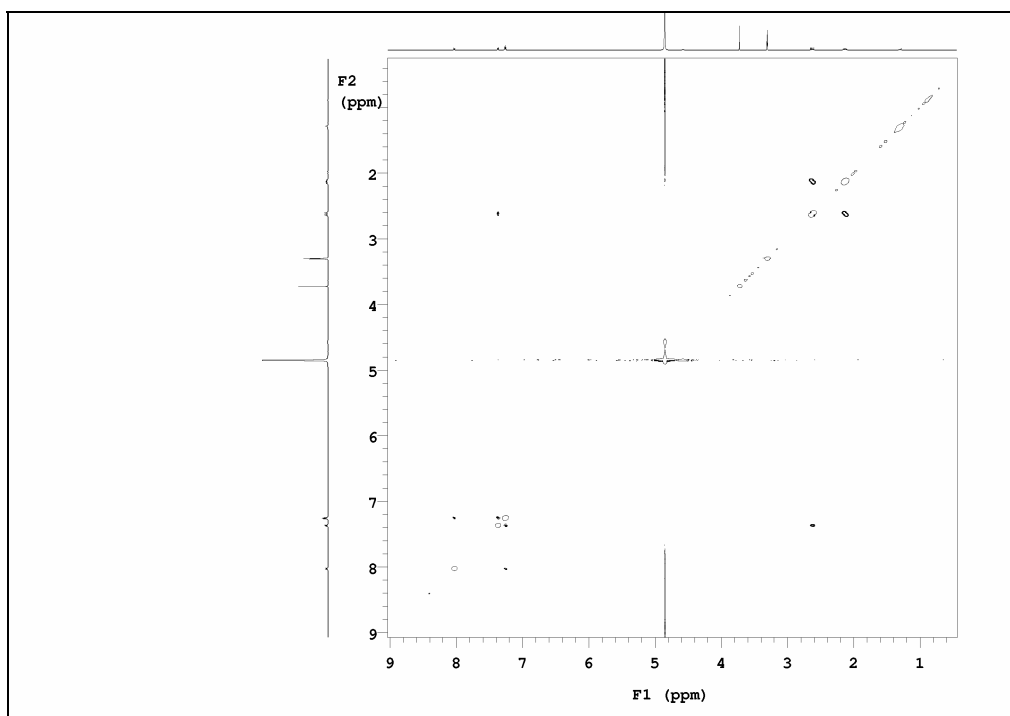
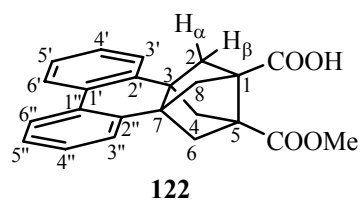
 $^1\text{H-RMN}$ (500 MHz, CD_3OD) $^{13}\text{C-RMN}$ (50.3 MHz, CDCl_3 + gotas CD_3OD)



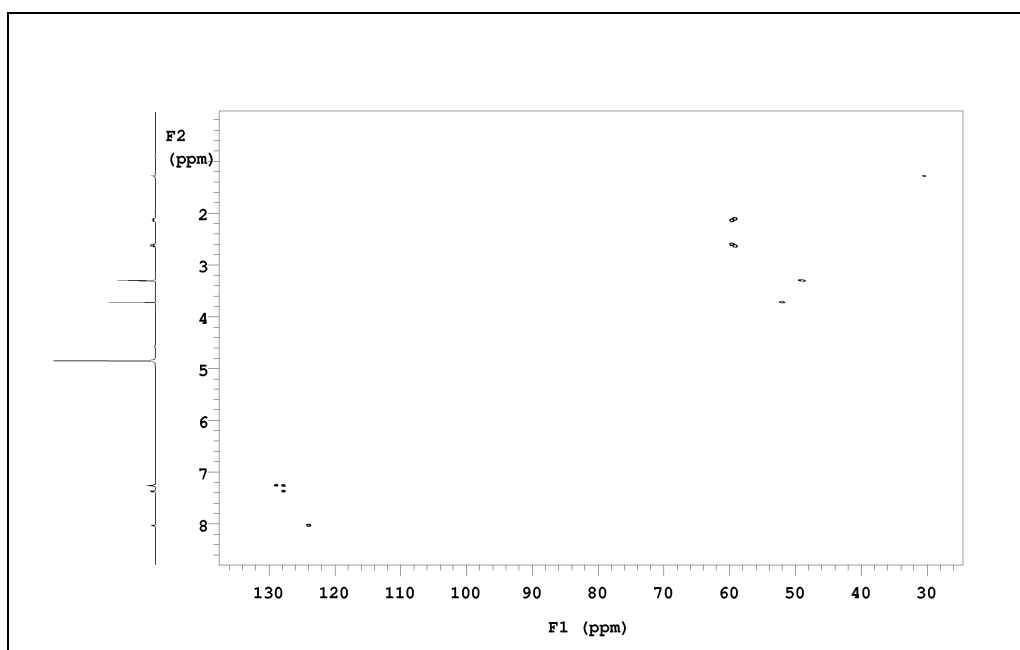
¹³C-DEPT



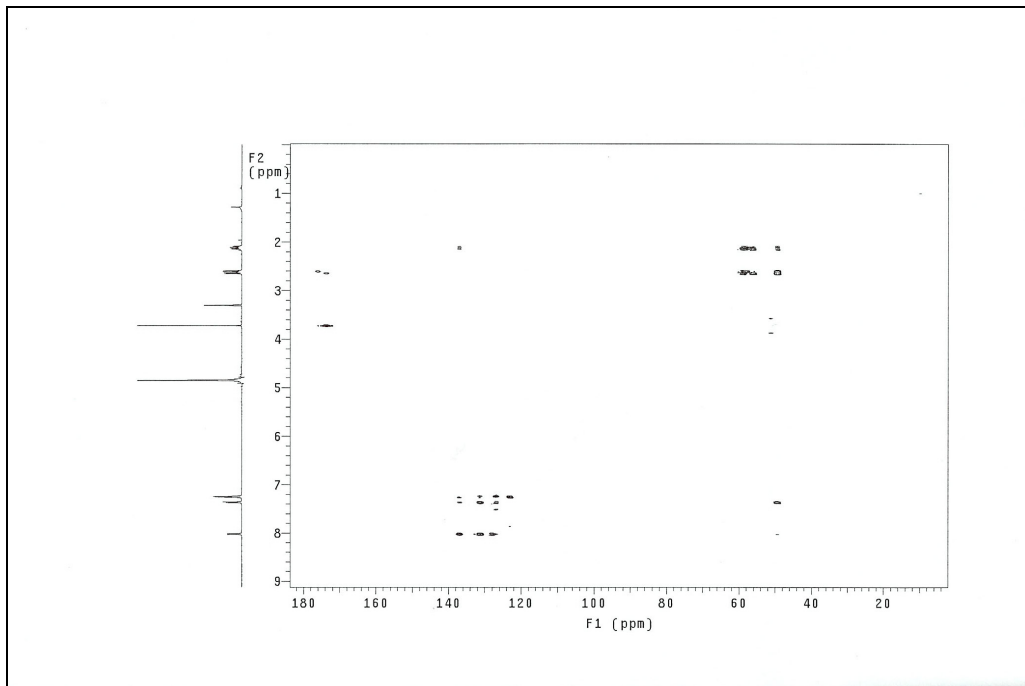
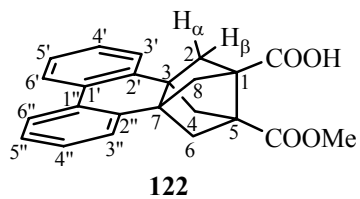
¹H-¹H-COSY



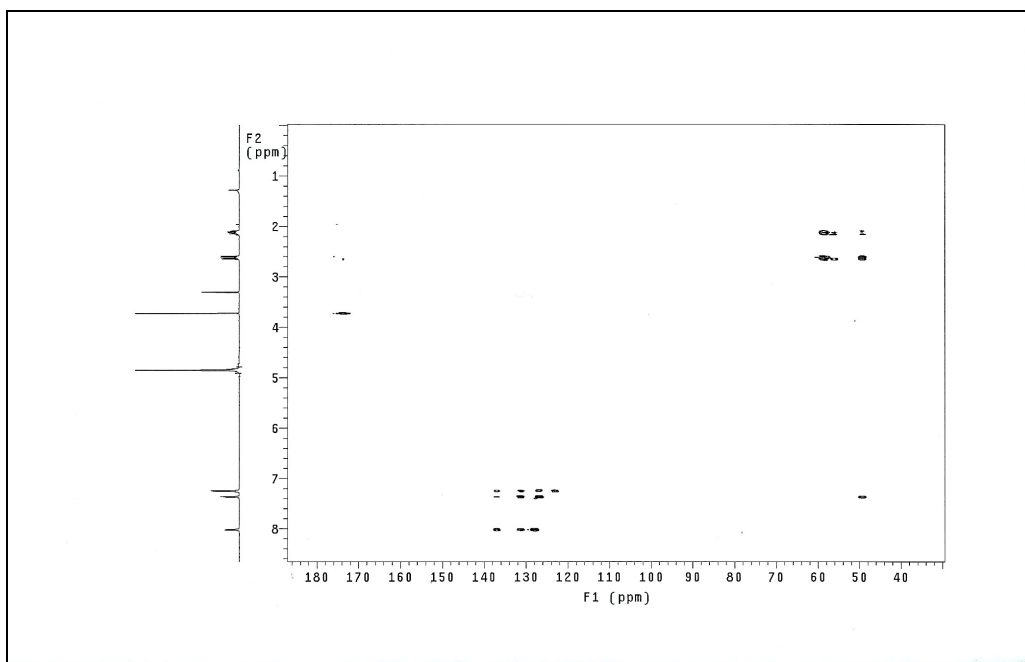
^1H - ^1H -NOESY



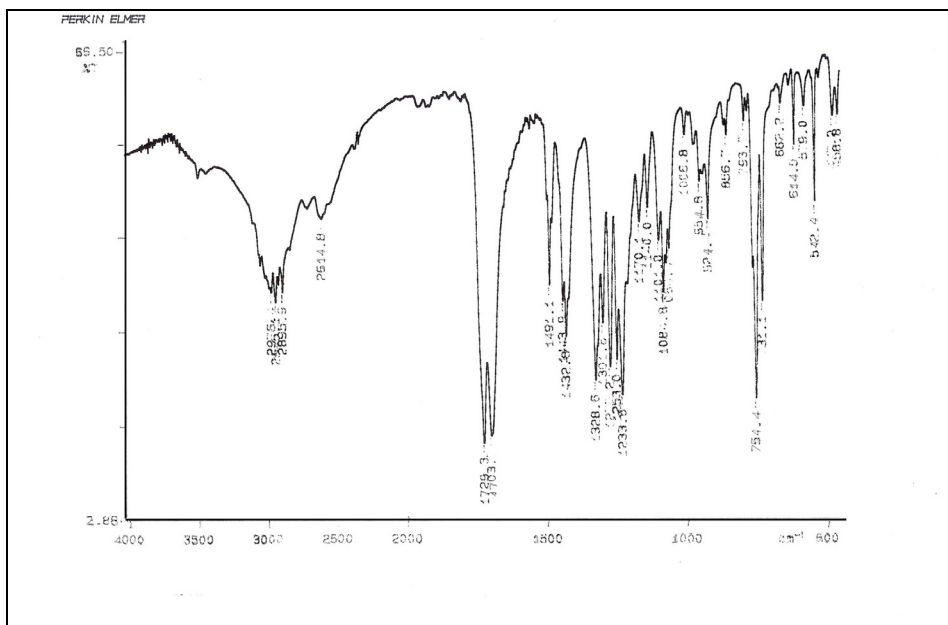
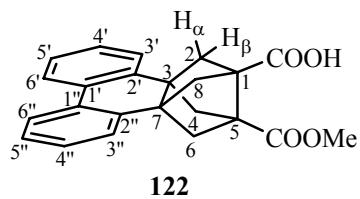
^1H - ^{13}C -HSQC



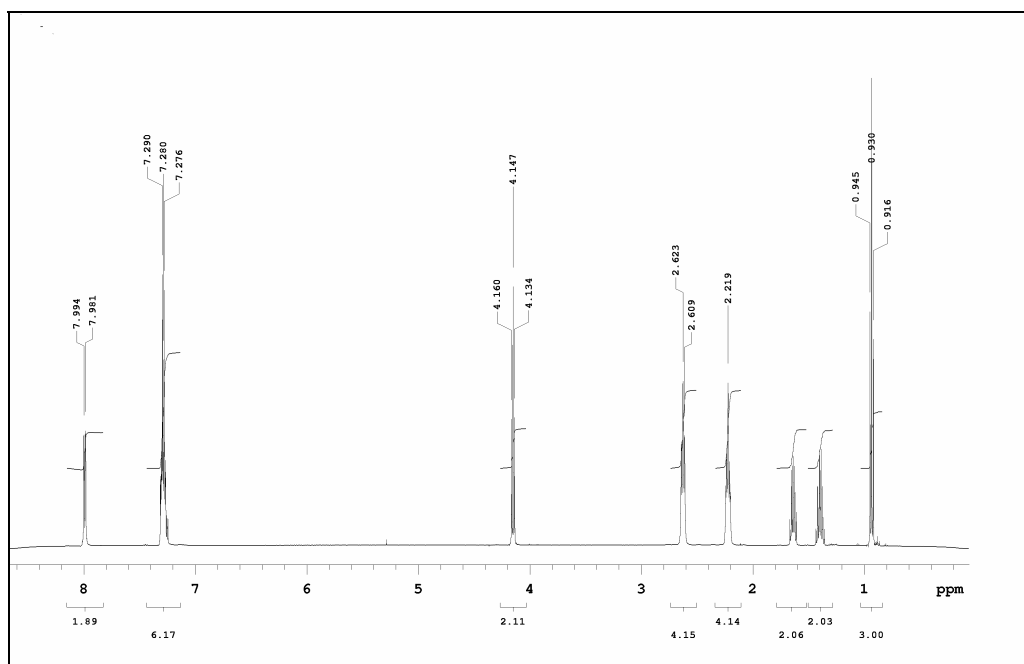
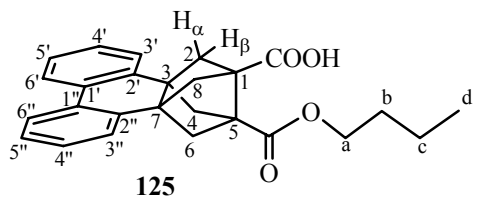
$^1\text{H}-^{13}\text{C}$ -HMBC $J = 8 \text{ Hz}$



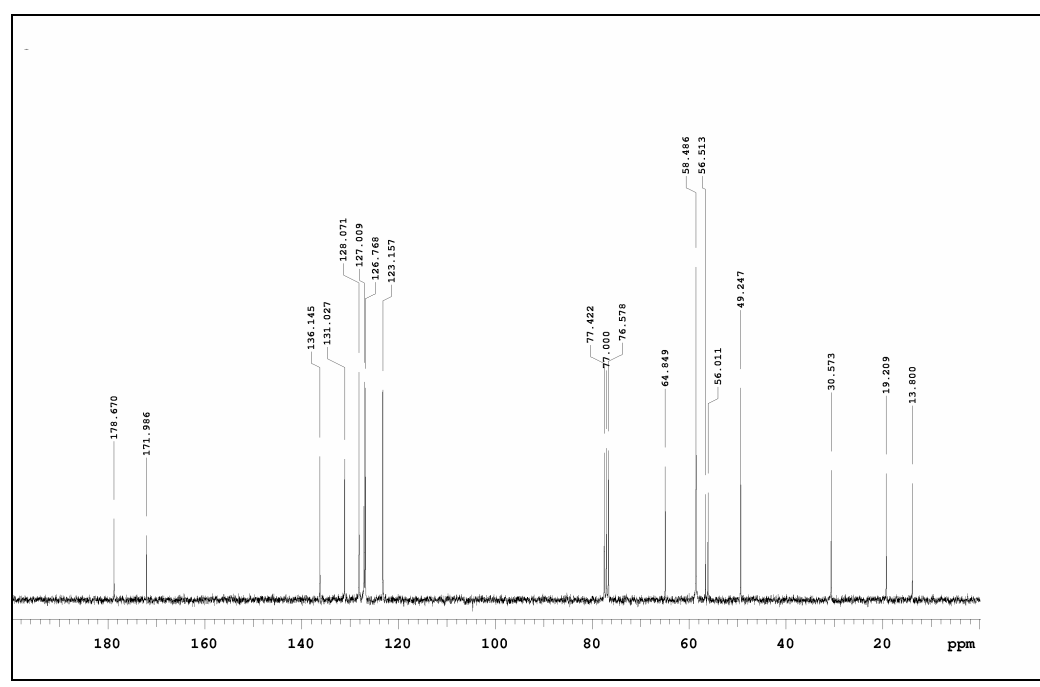
$^1\text{H}-^{13}\text{C}$ -HMBC $J = 5 \text{ Hz}$



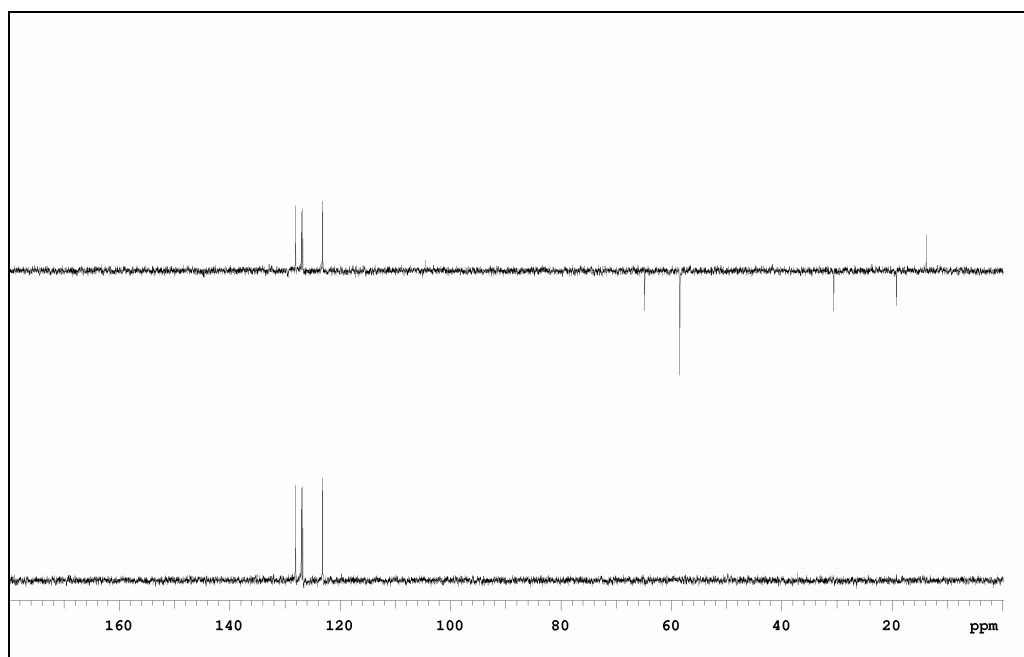
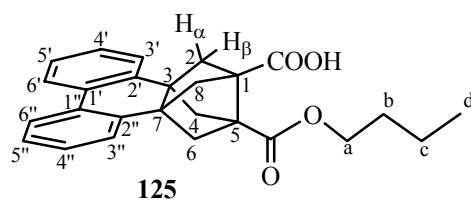
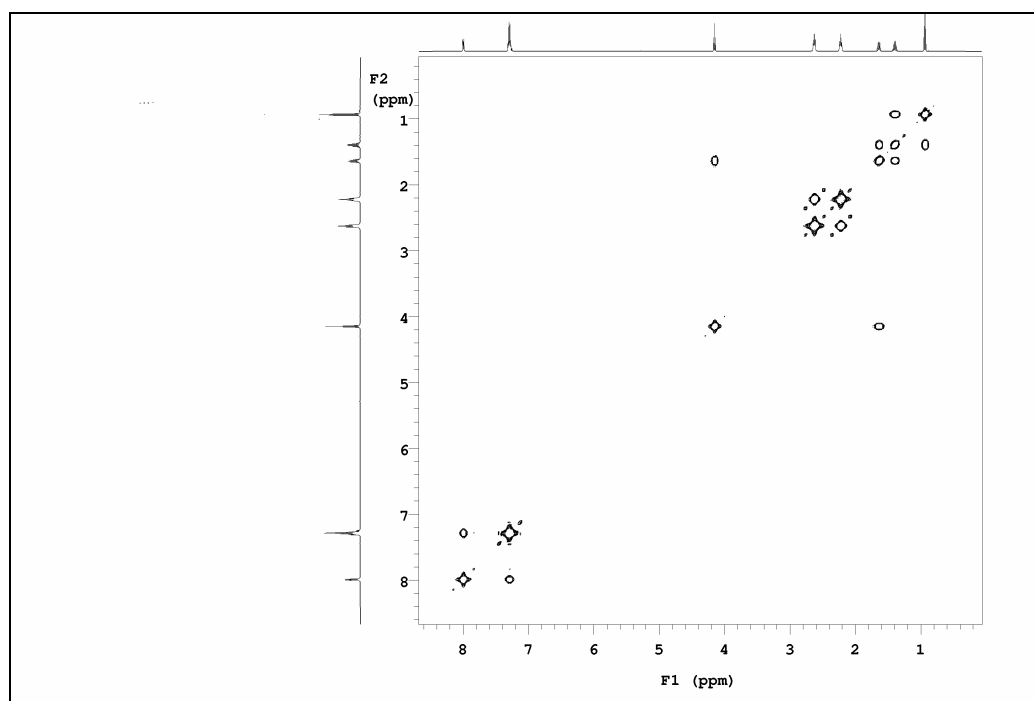
IR (KBr)

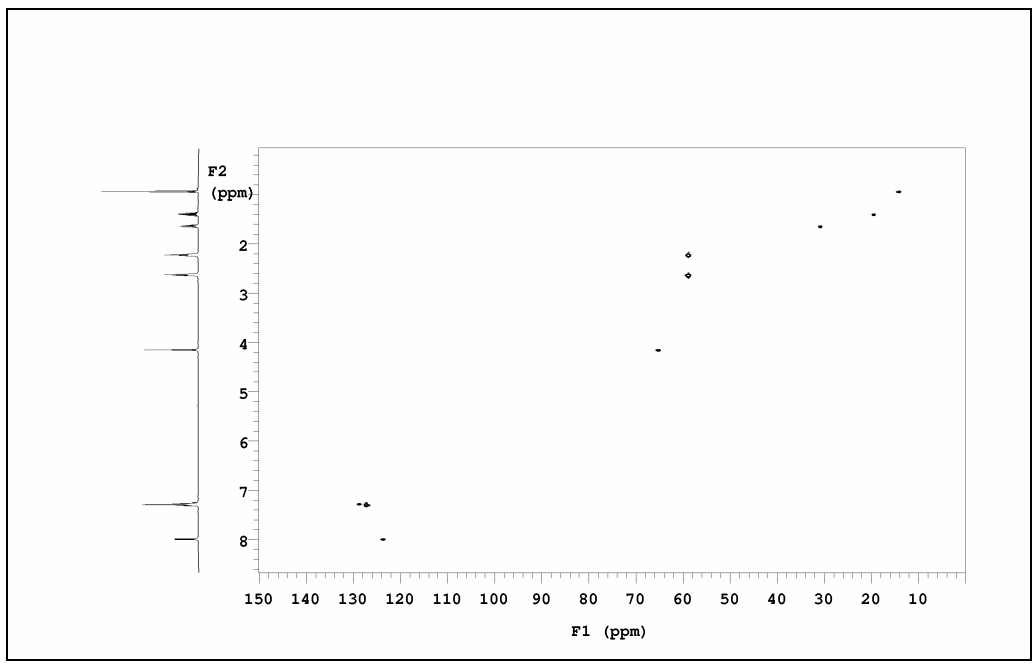
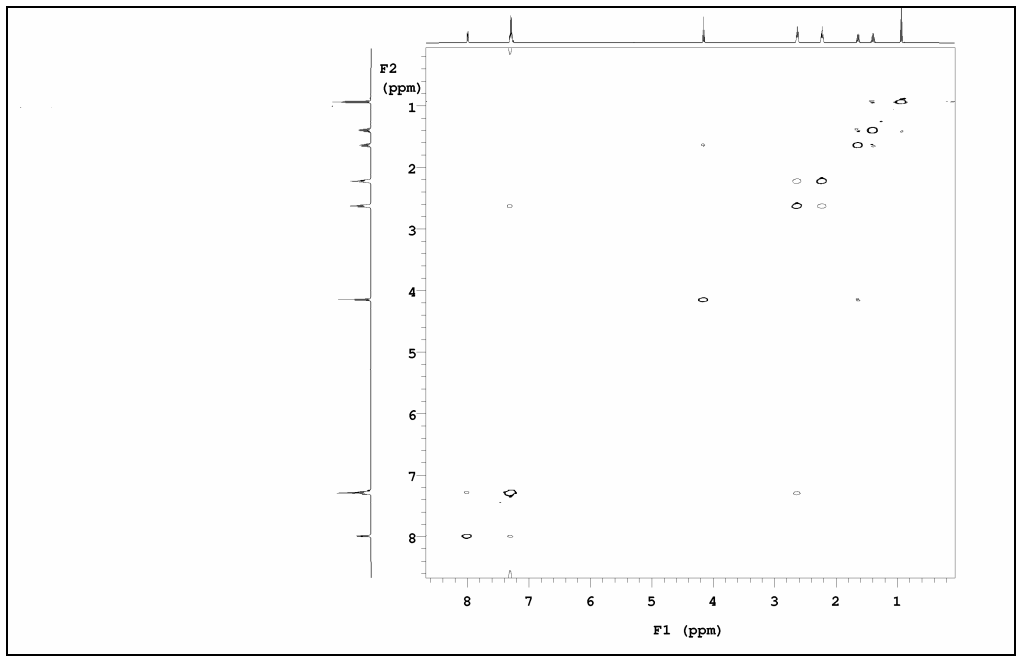
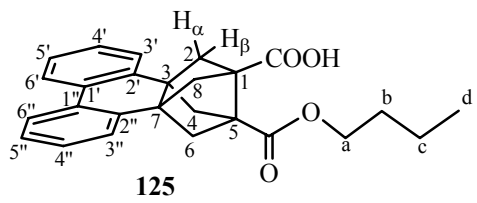


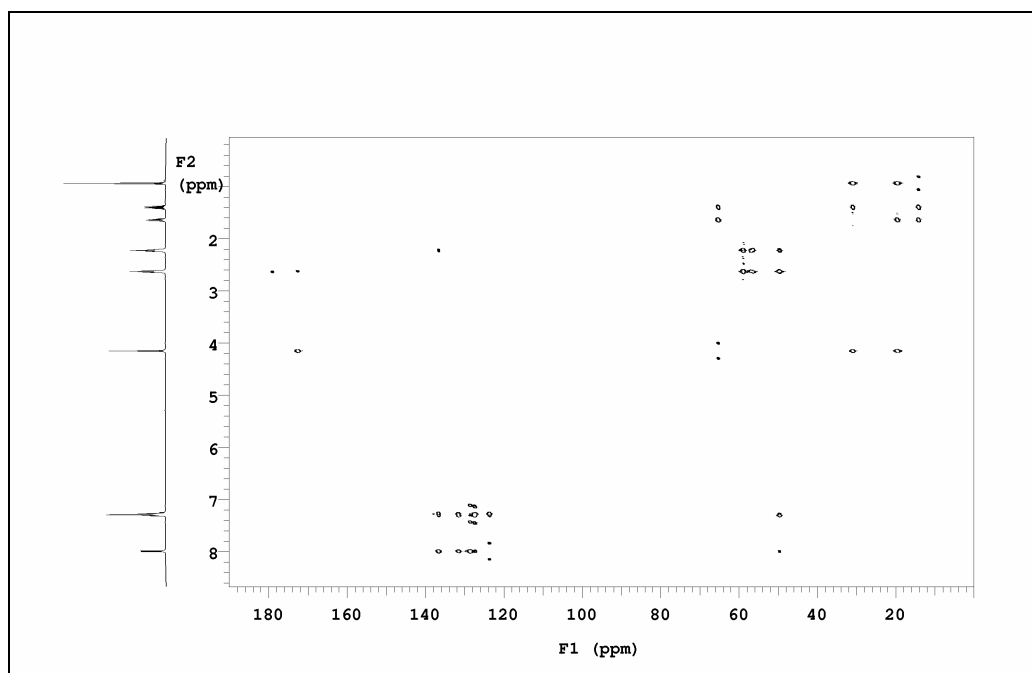
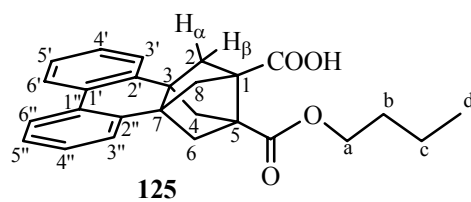
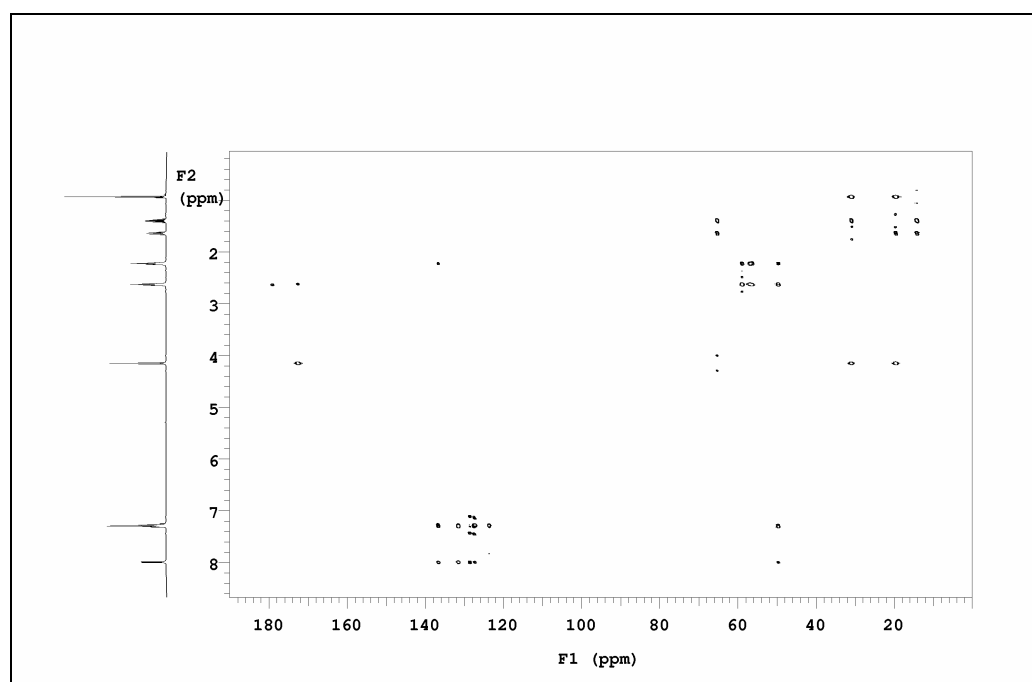
¹H-RMN (500 MHz, CDCl₃)

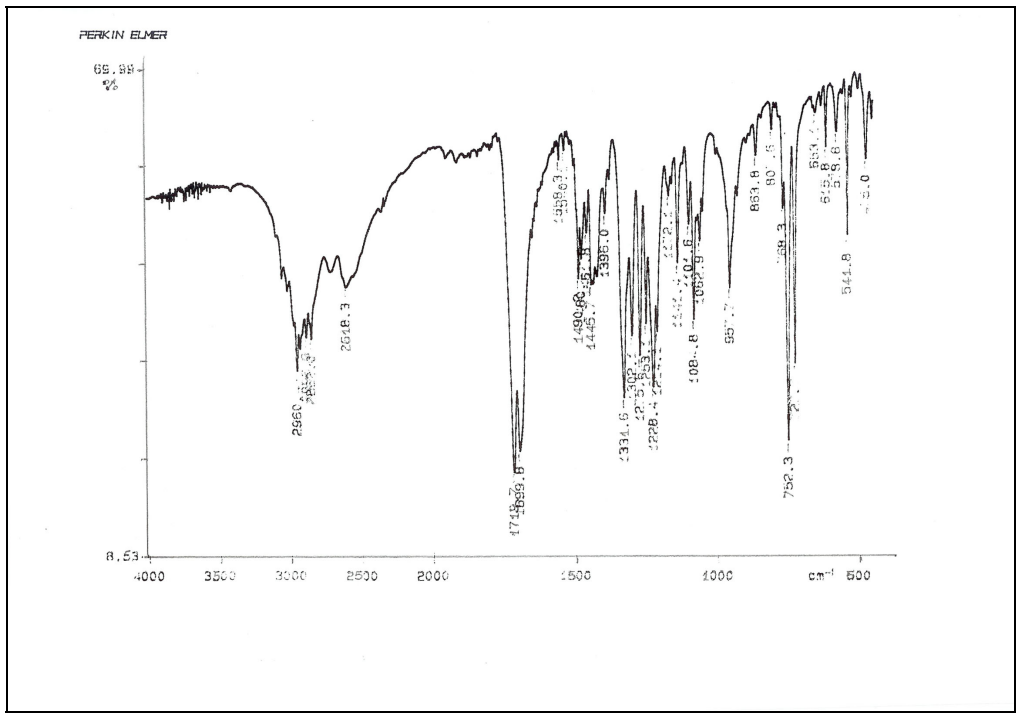
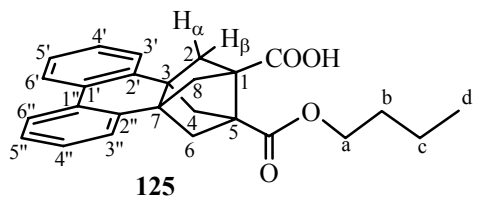


¹³C-RMN (75.4 MHz, CDCl₃)

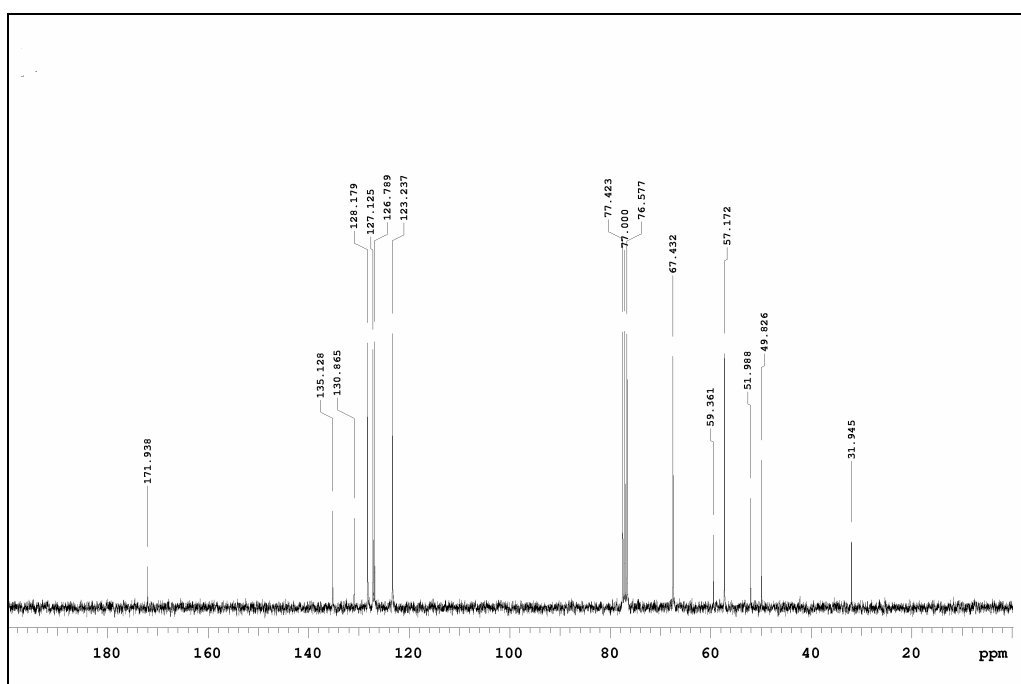
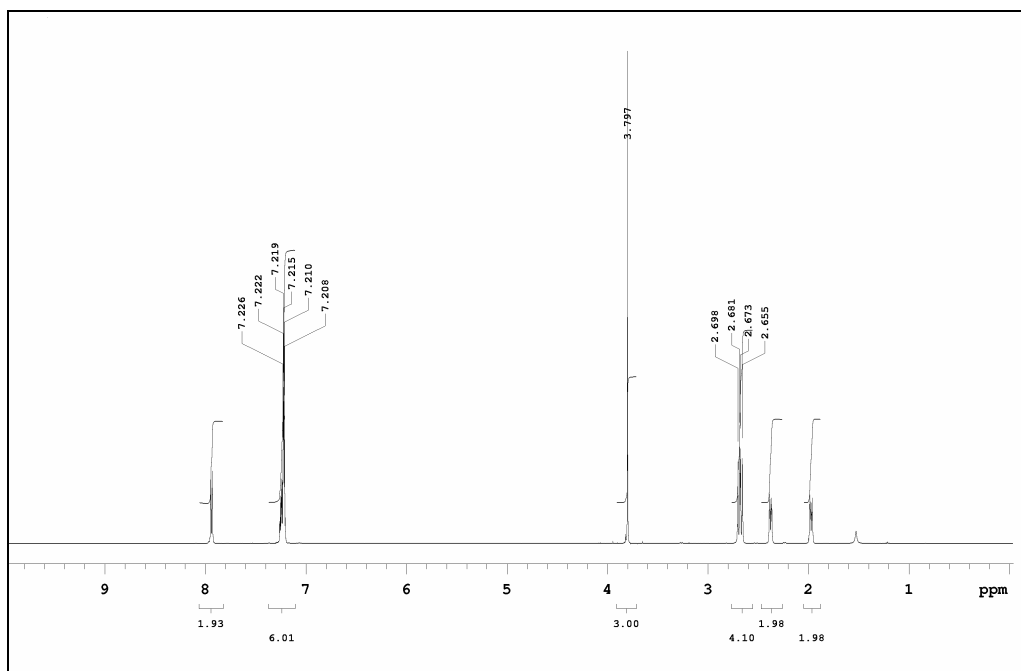
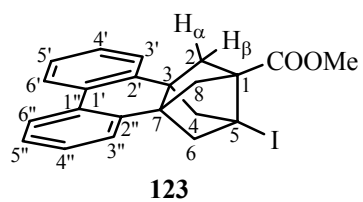
 ^{13}C -DEPT ^1H - ^1H -COSY

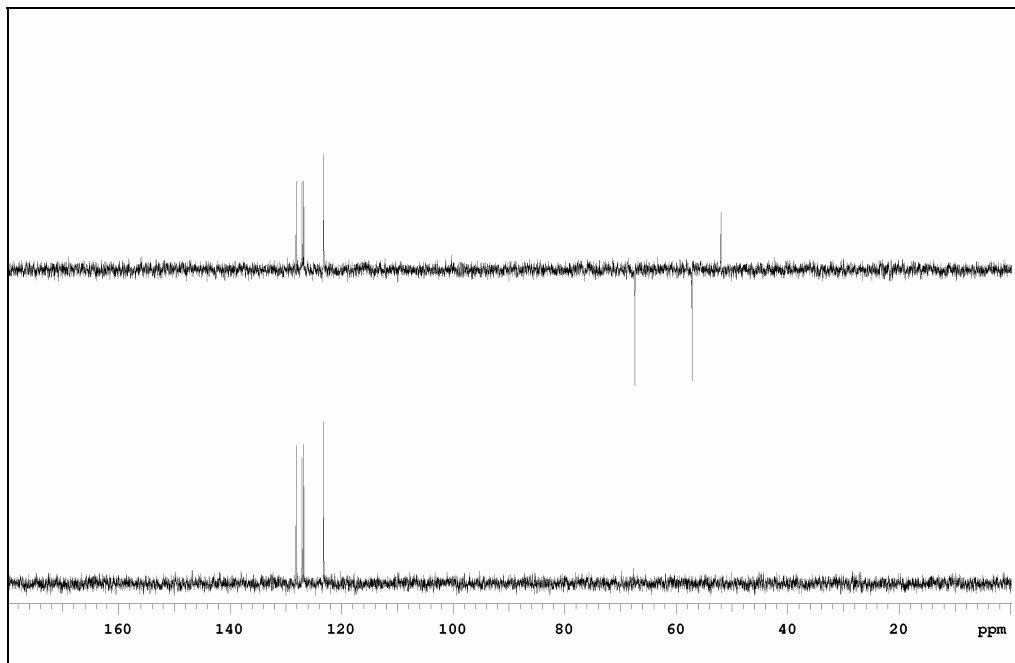
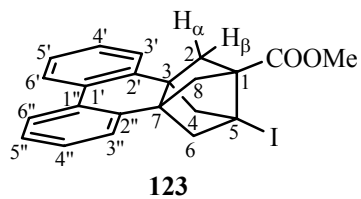


 $^1\text{H}-^{13}\text{C}$ -HMBC J = 60 ms $^1\text{H}-^{13}\text{C}$ -HMBC J = 110 ms

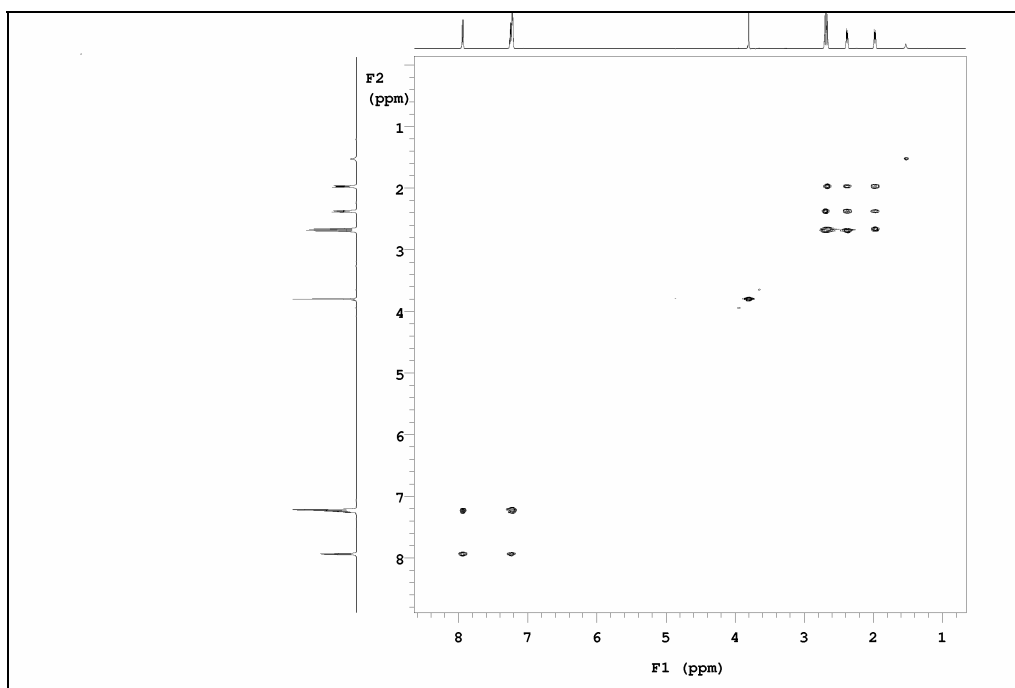


IR (KBr)

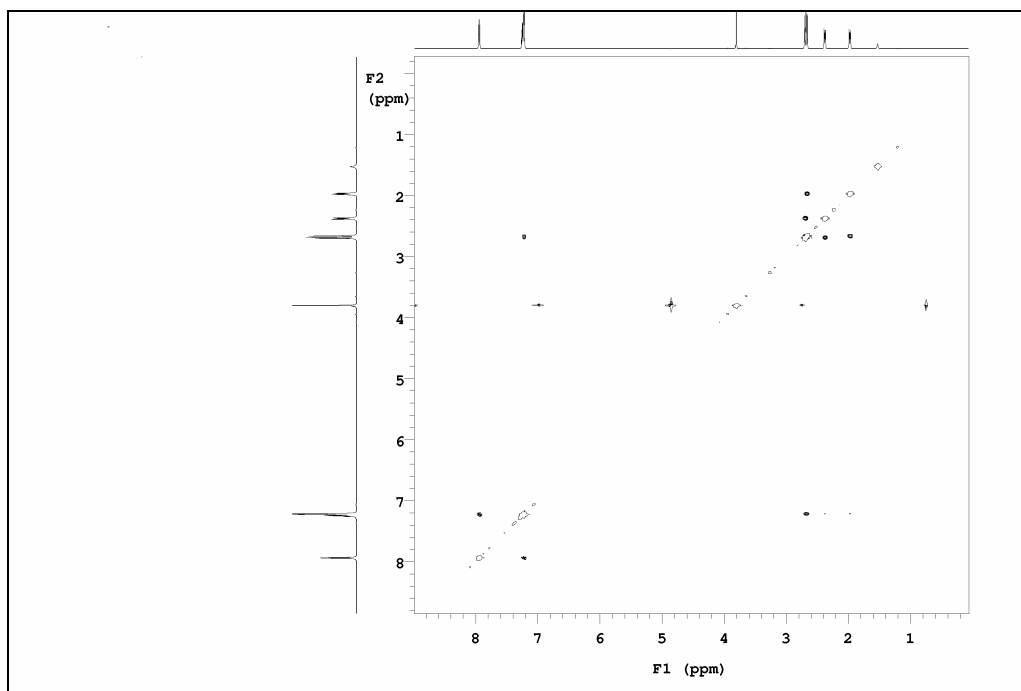
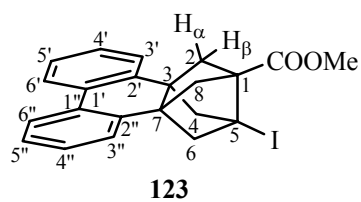




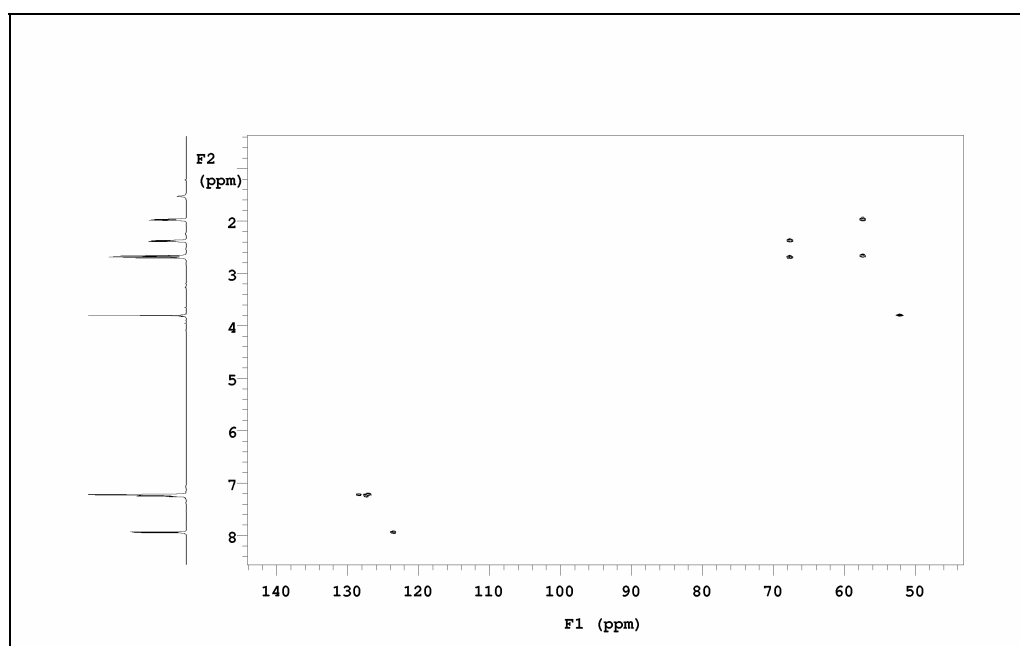
^{13}C -DEPT



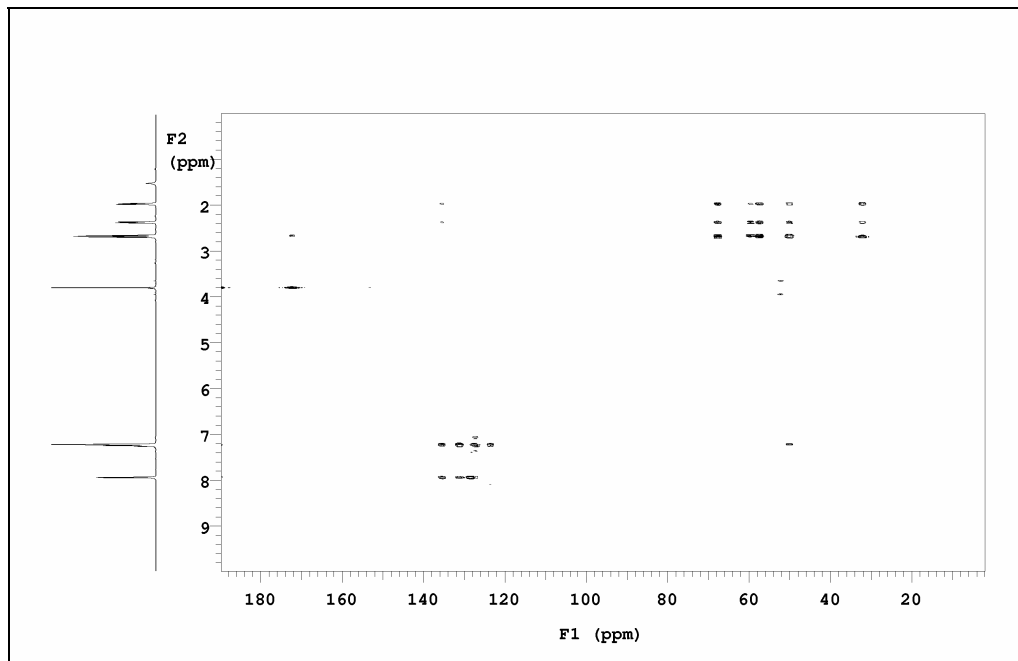
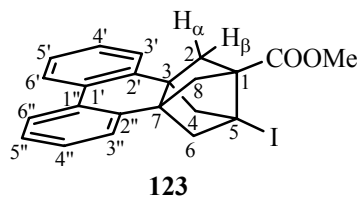
^1H - ^1H -COSY



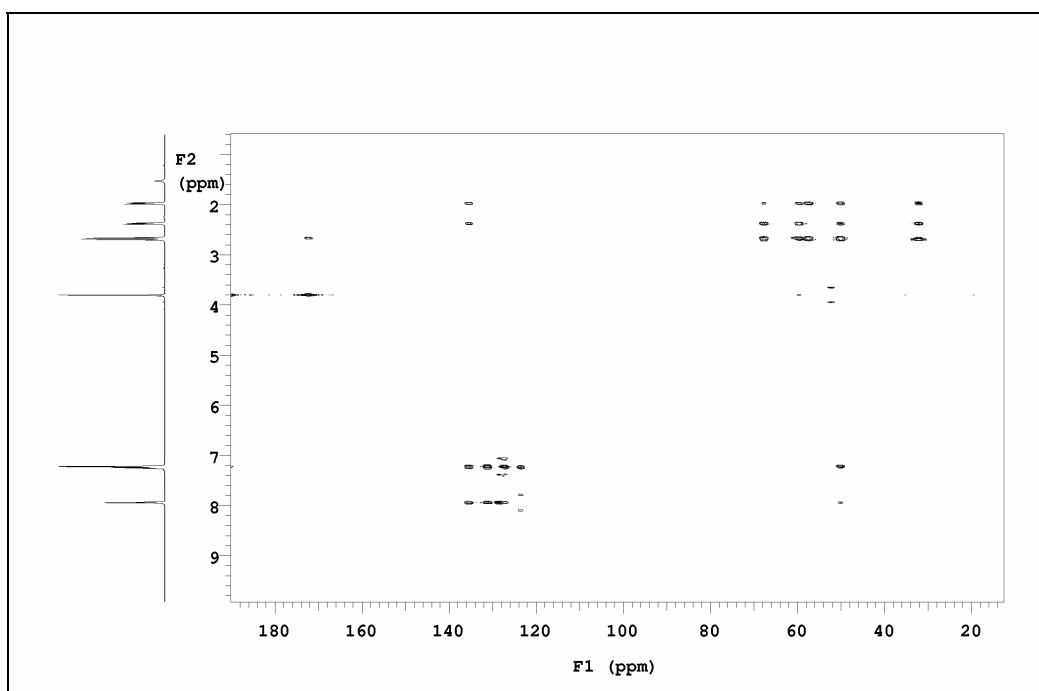
$^1\text{H}-^1\text{H}$ -NOESY



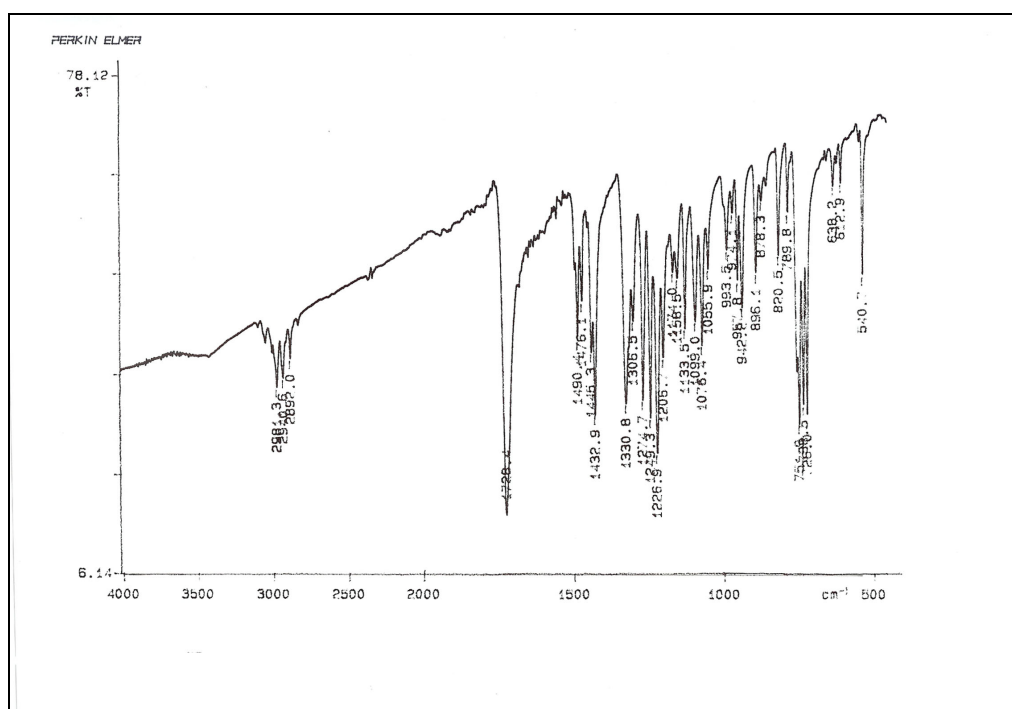
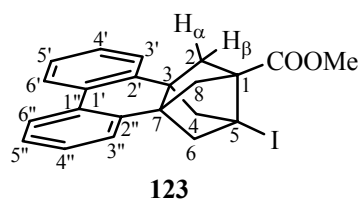
$^1\text{H}-^{13}\text{C}$ -HSQC



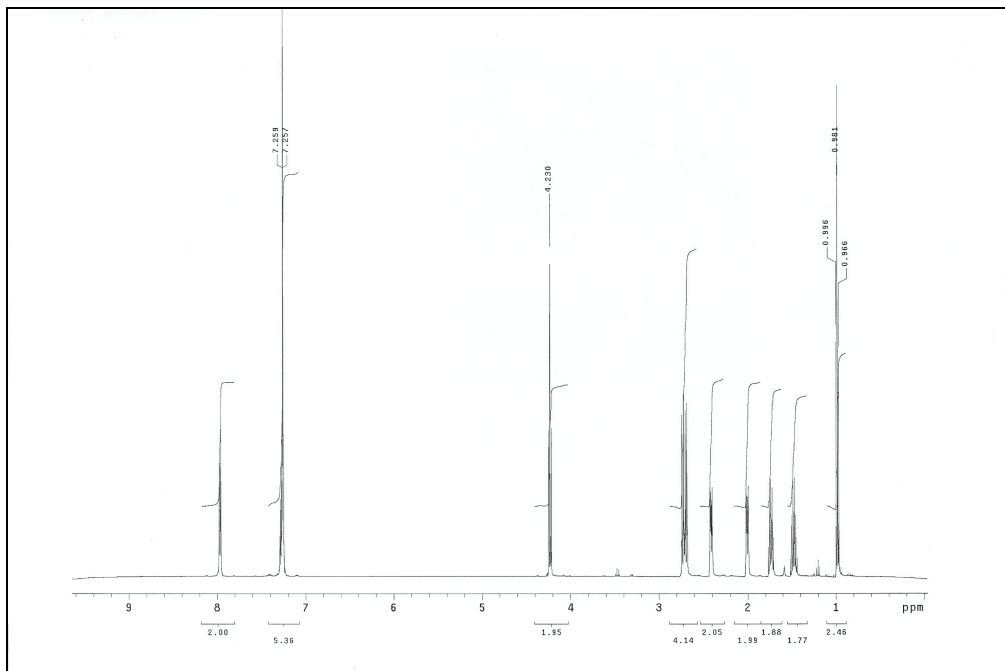
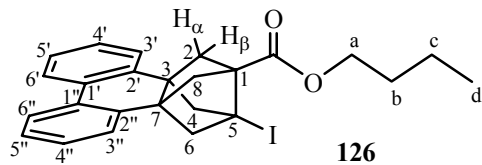
$^1\text{H}-^{13}\text{C}$ -HMBC $J = 8 \text{ Hz}$



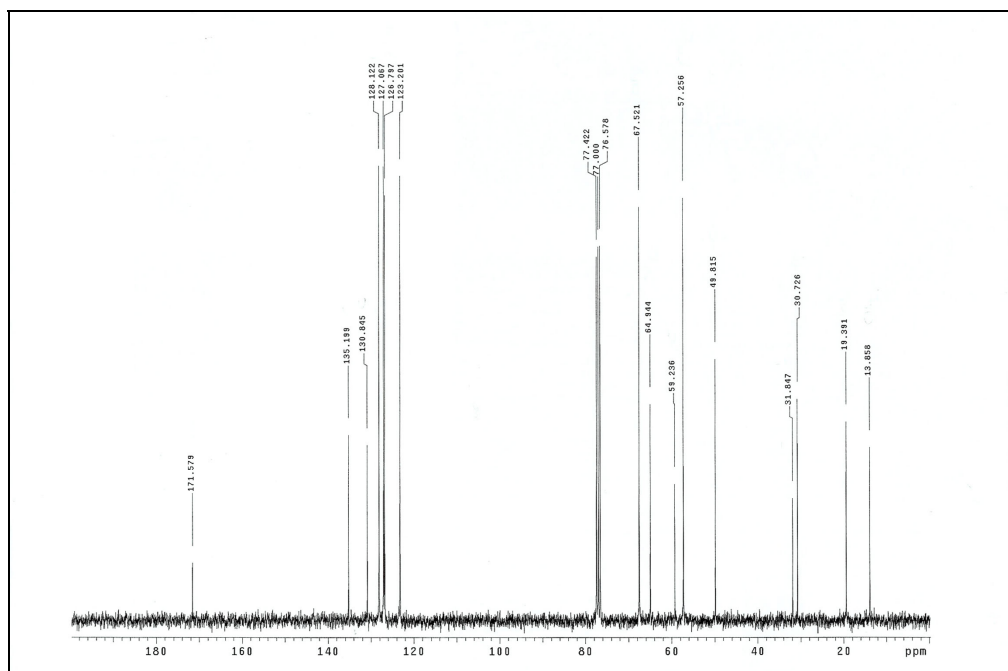
$^1\text{H}-^{13}\text{C}$ -HMBC $J = 5 \text{ Hz}$



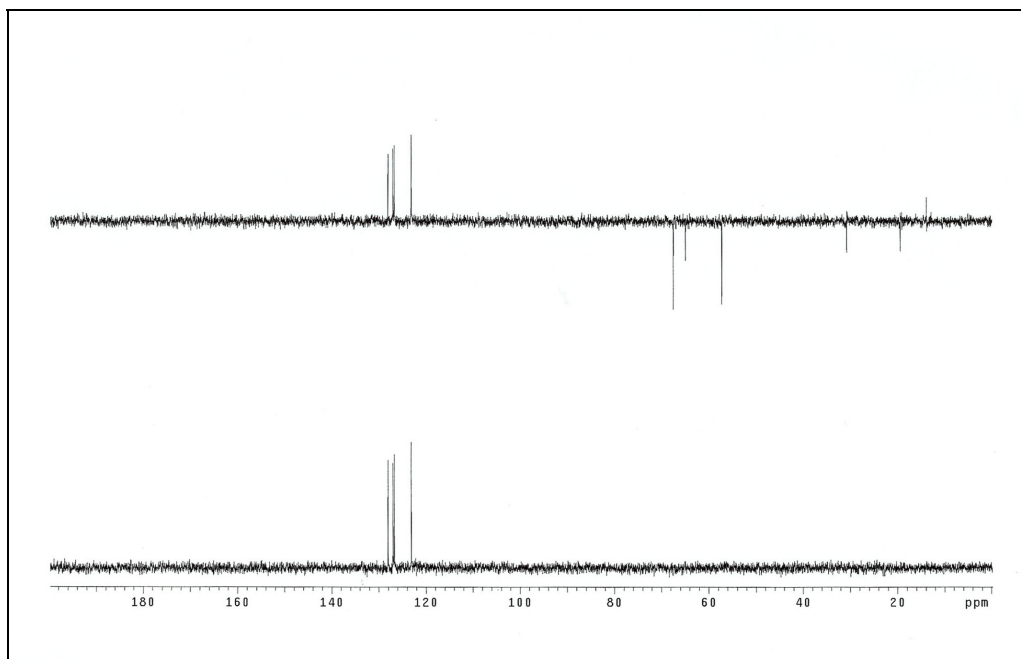
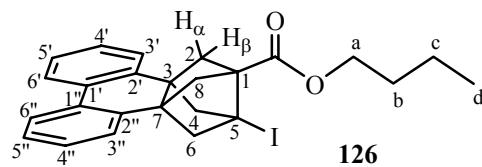
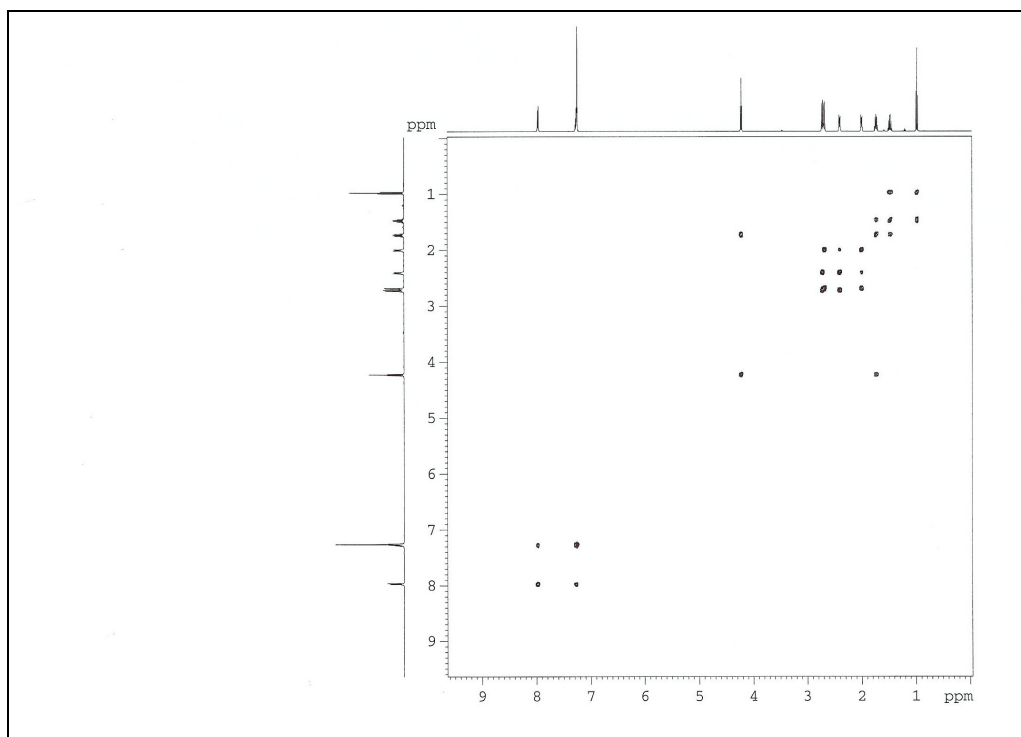
IR (KBr)

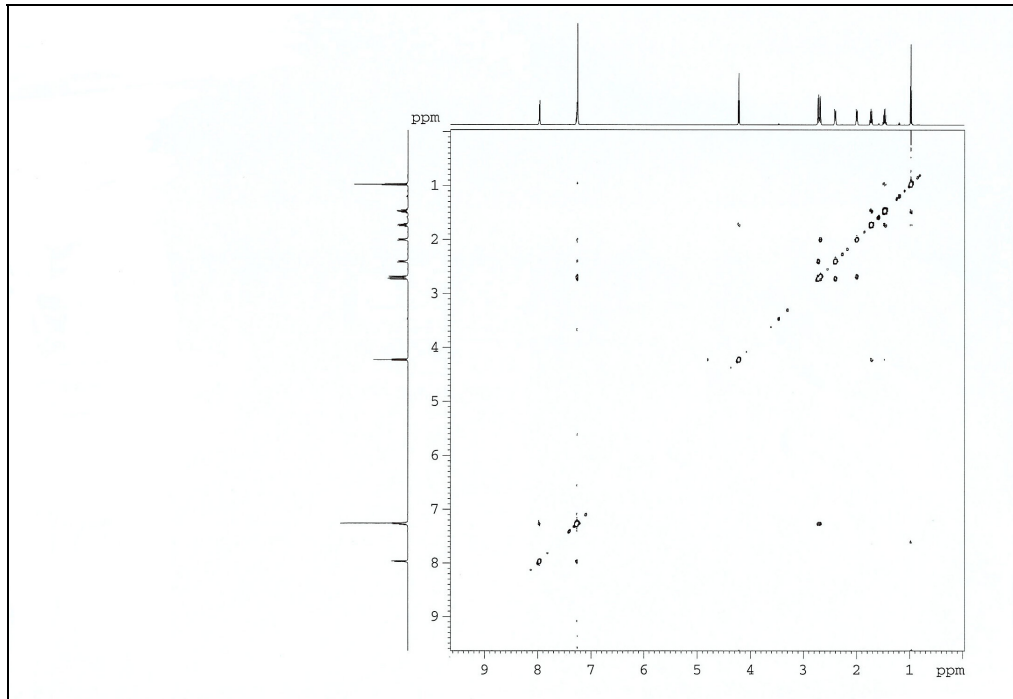
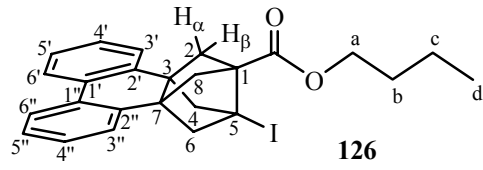


¹H-RMN (500 MHz, CDCl₃)

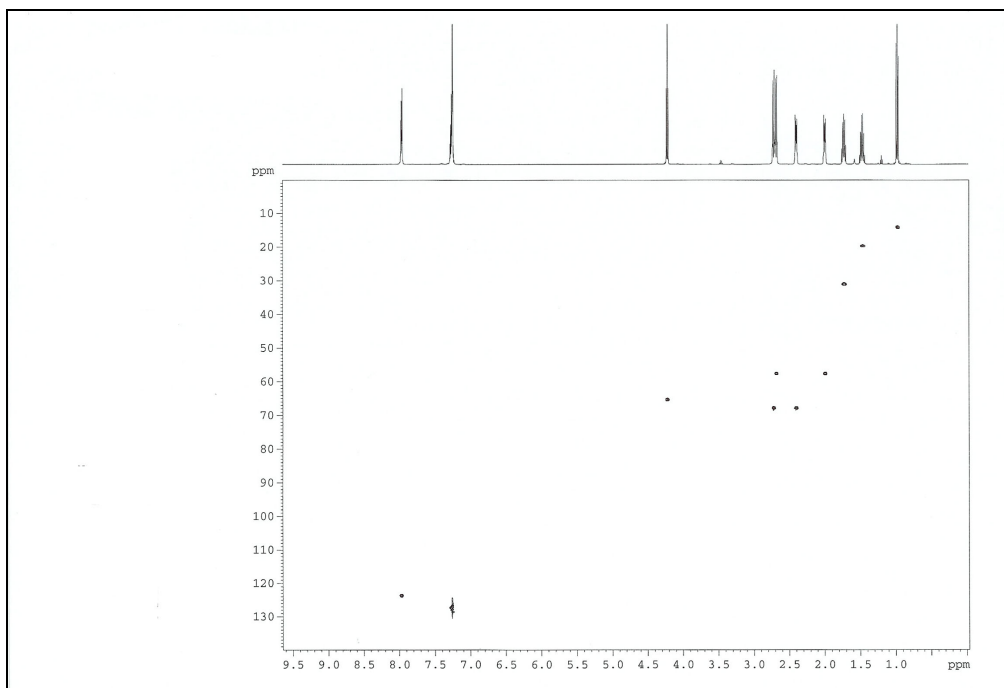


¹³C-RMN (75.4 MHz, CDCl₃)

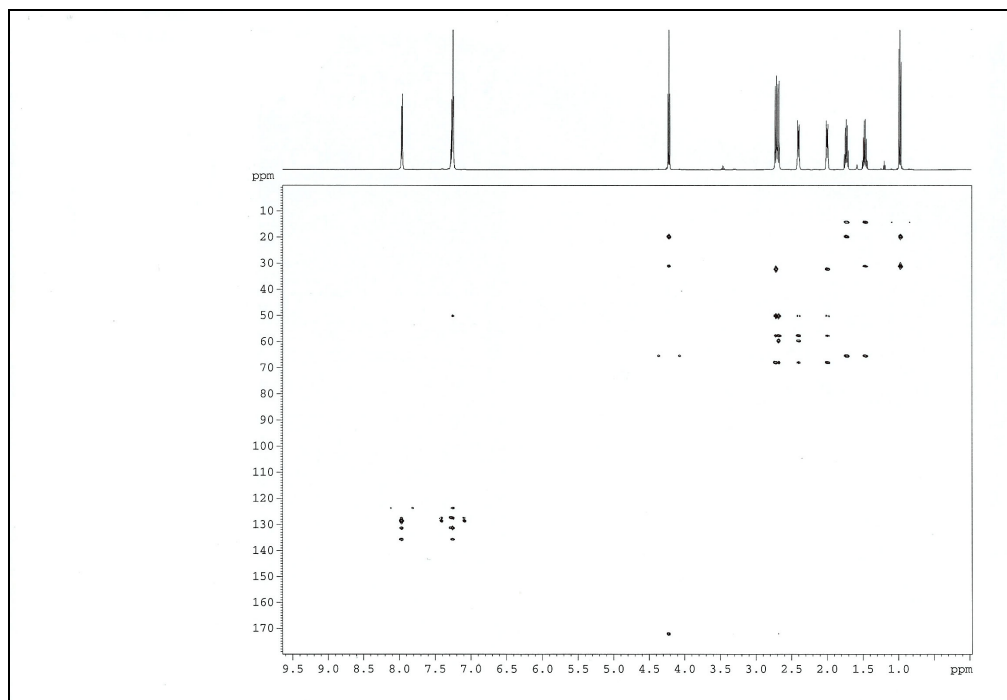
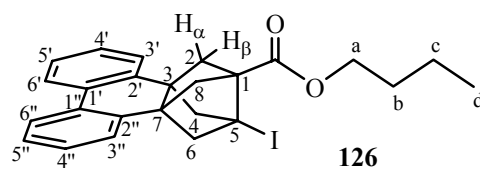
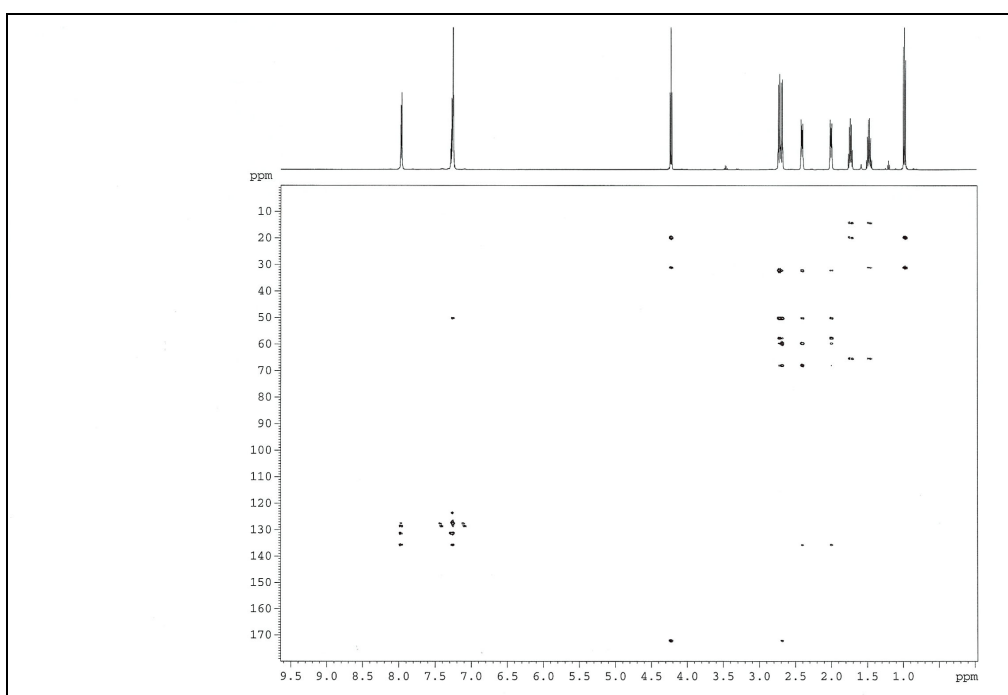
 ^{13}C -DEPT ^1H - ^1H -COSY

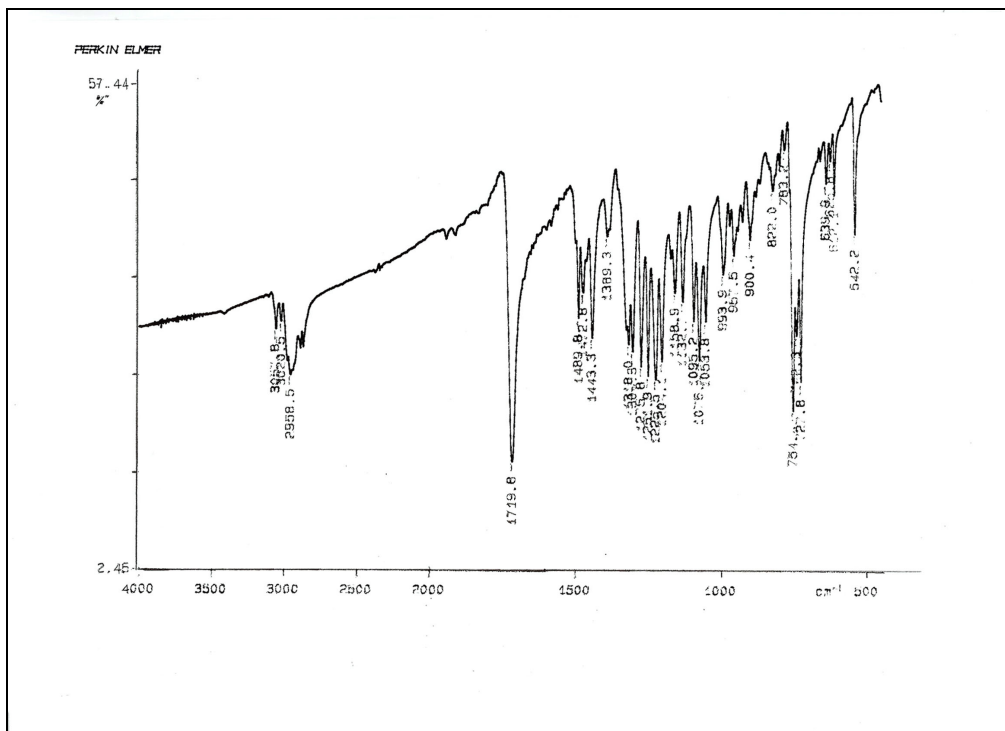
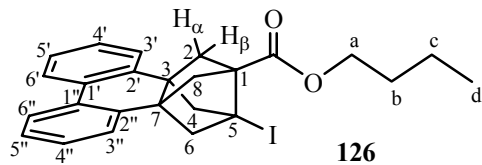


$^1\text{H}-^1\text{H}$ -NOESY

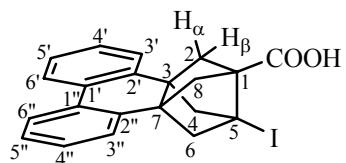


$^1\text{H}-^{13}\text{C}$ -HSQC

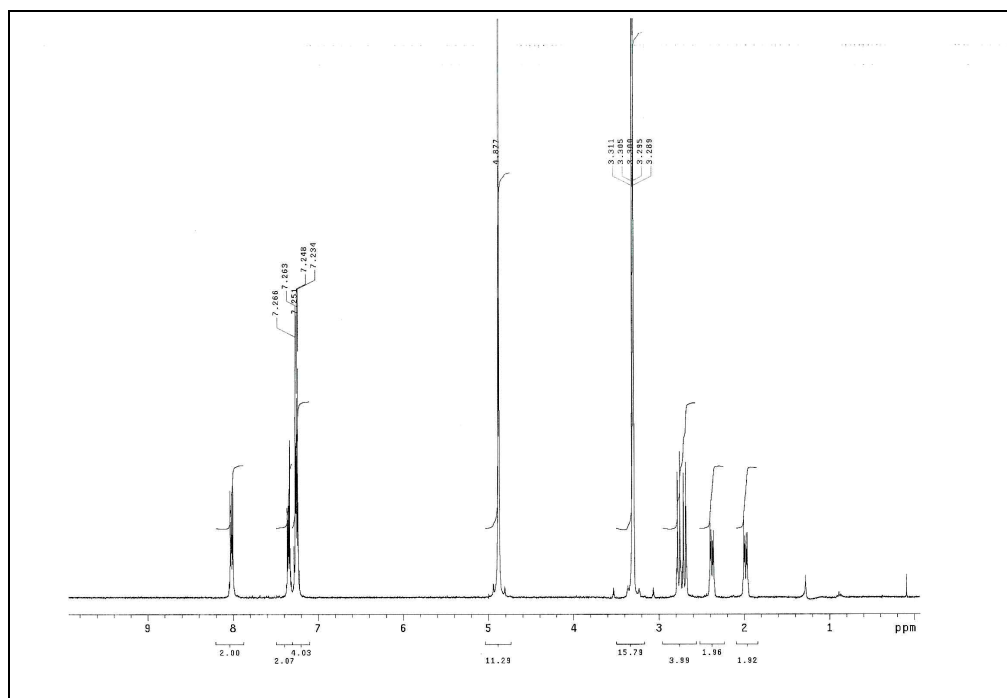
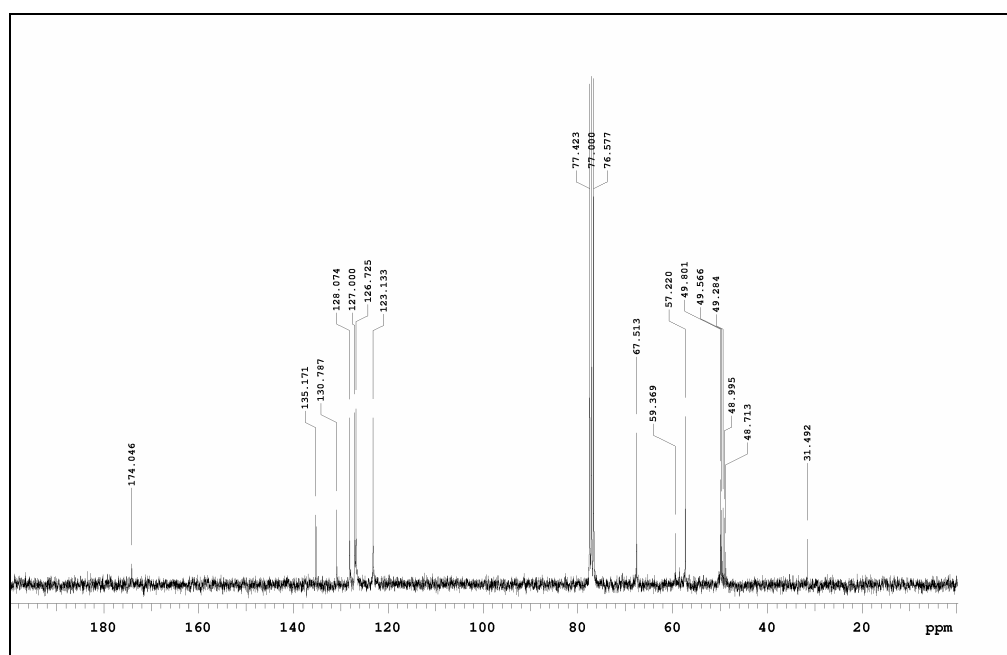
 $^1\text{H}-^{13}\text{C}\text{-HMBC } J = 60 \text{ ms}$  $^1\text{H}-^{13}\text{C}\text{-HMBC } J = 110 \text{ ms}$

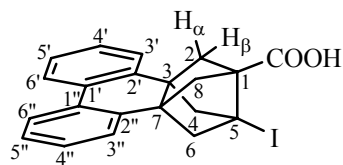


IR (KBr)

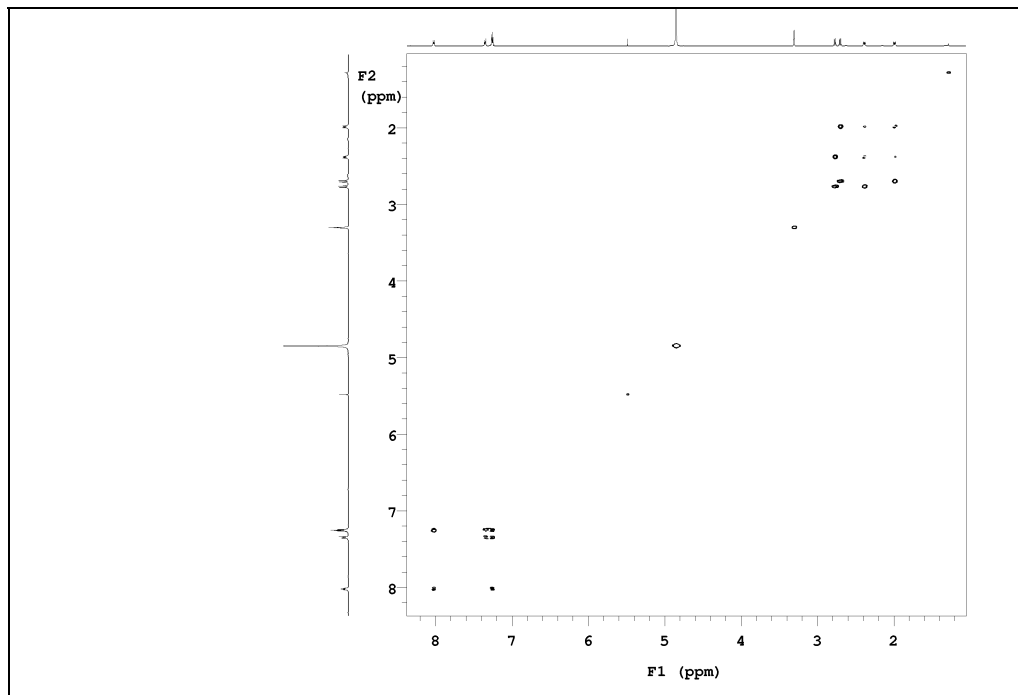


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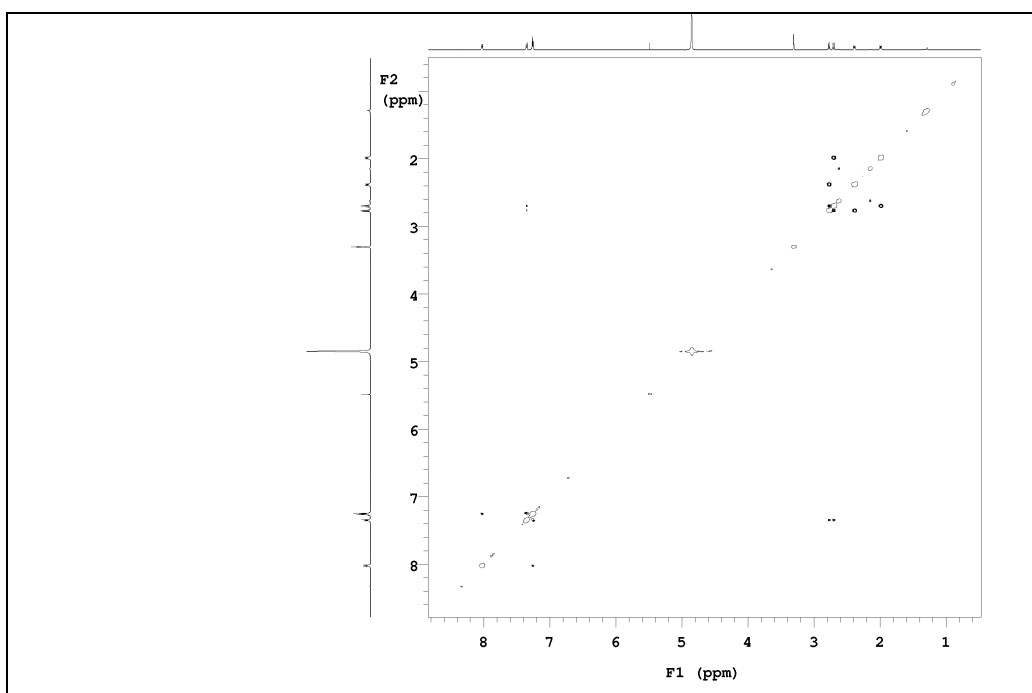
 $^1\text{H-RMN}$ (500 MHz, CDCl_3) $^{13}\text{C-RMN}$ (75.4 MHz, CDCl_3)



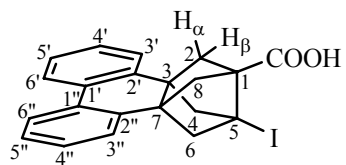
124



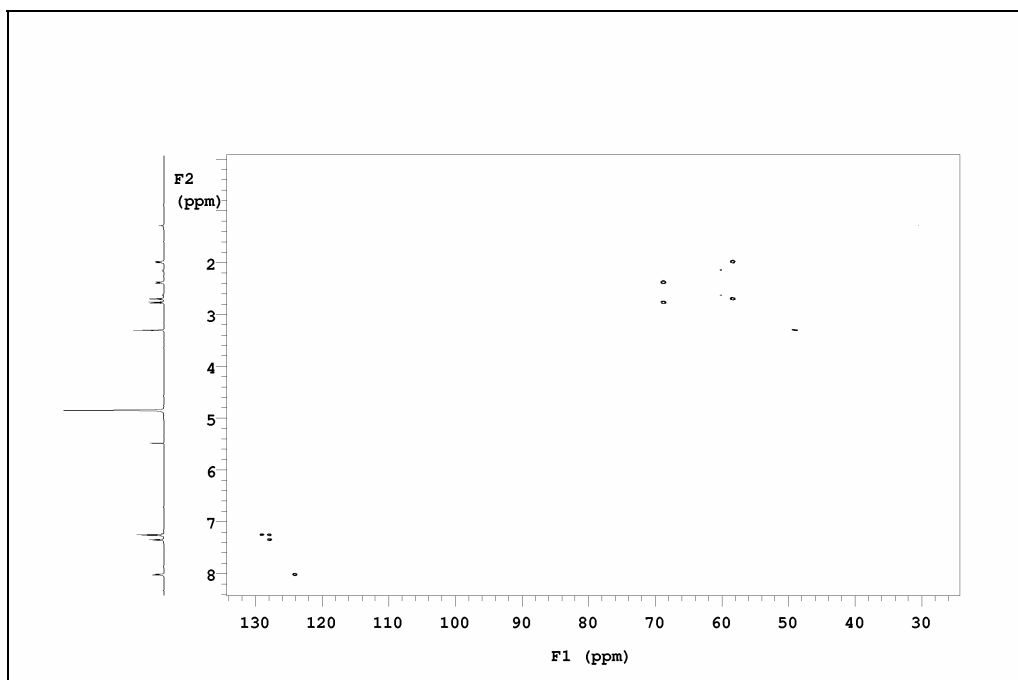
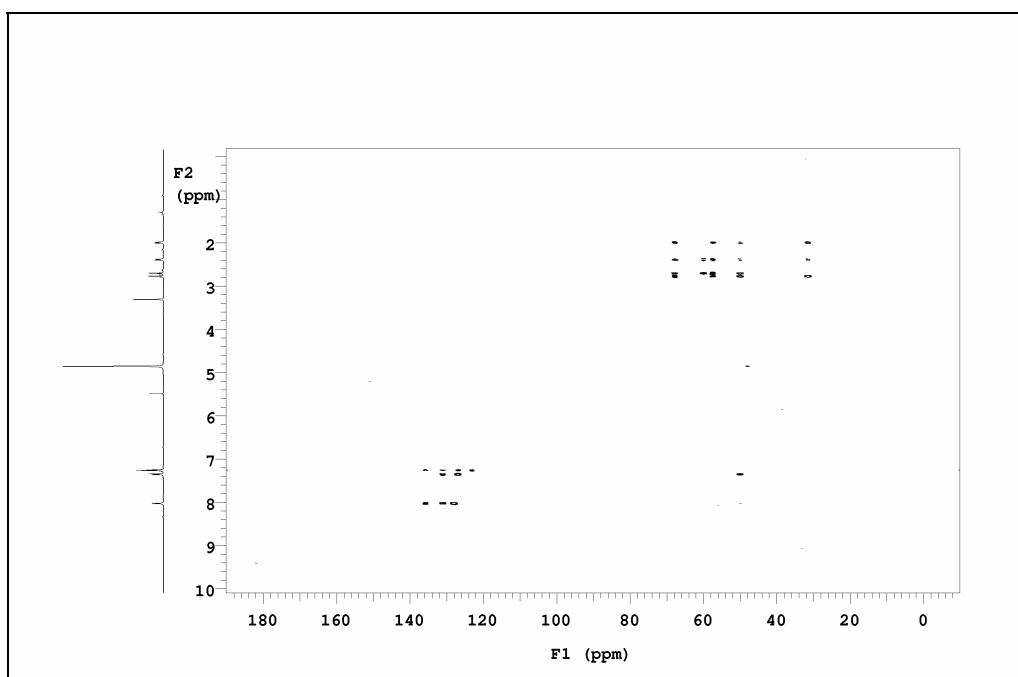
$^1\text{H}-^1\text{H}$ -COSY

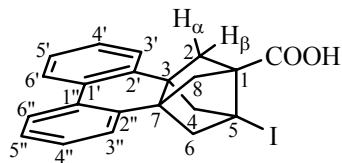


$^1\text{H}-^1\text{H}$ -NOESY

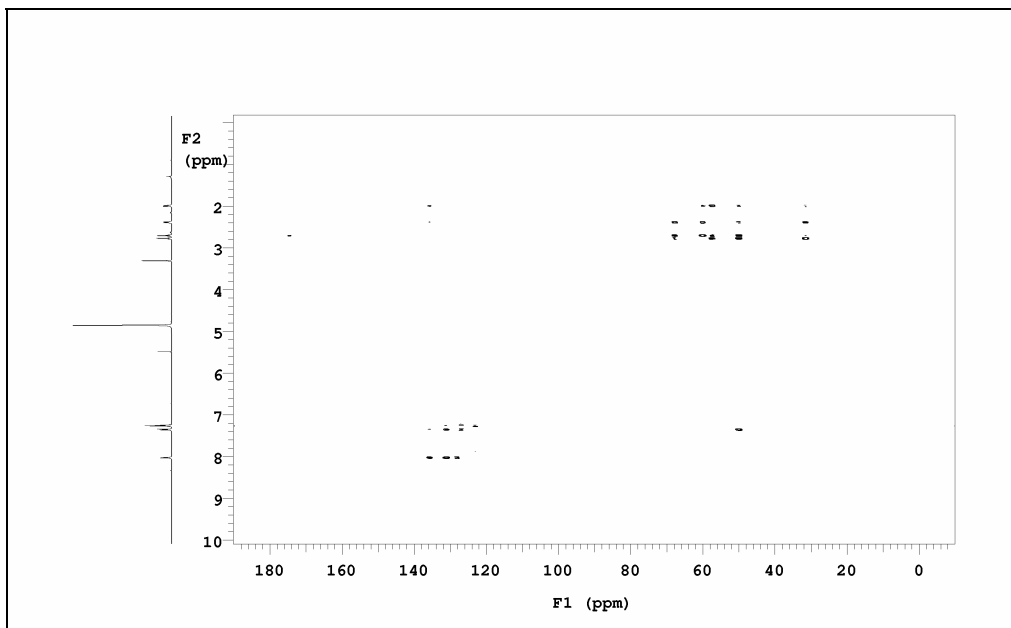


124

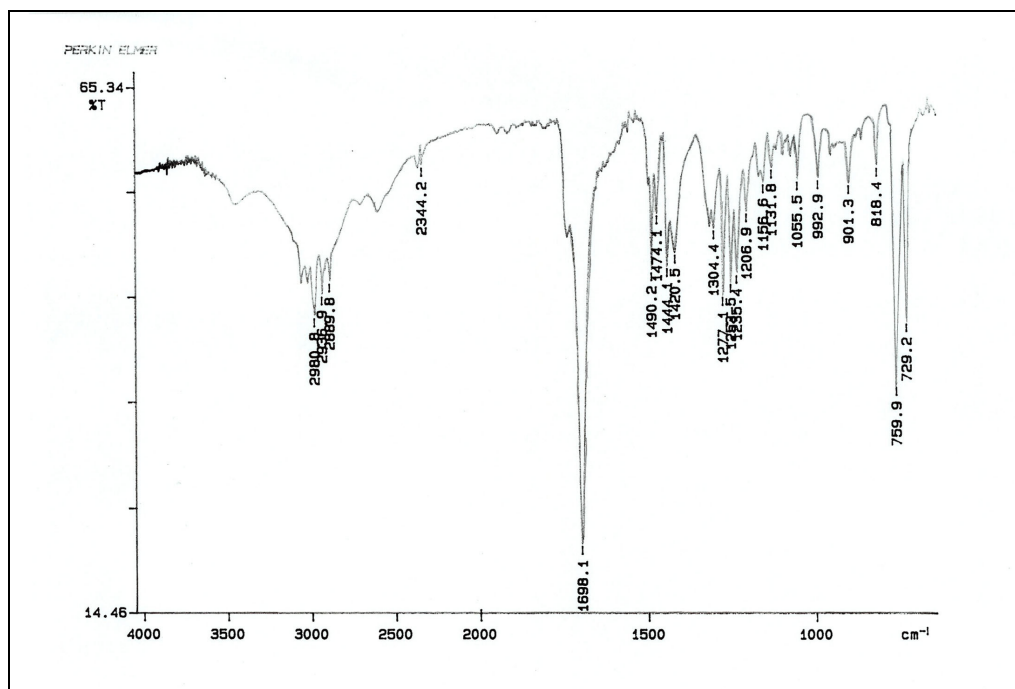
 ^1H - ^{13}C -HSQC ^1H - ^{13}C -HMBC $J = 8$ Hz



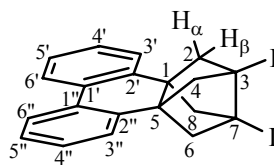
124



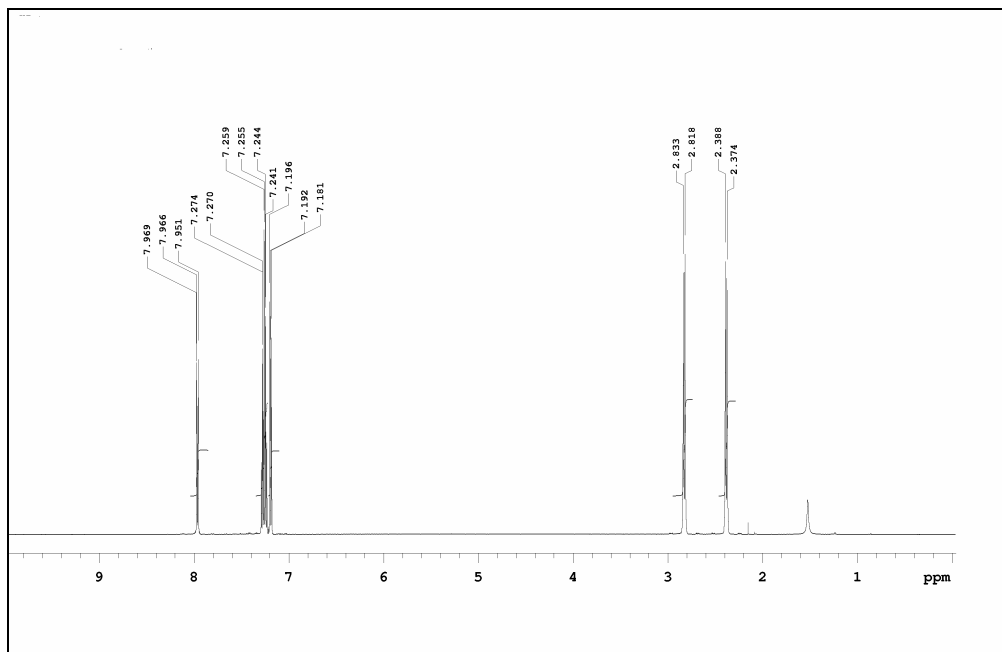
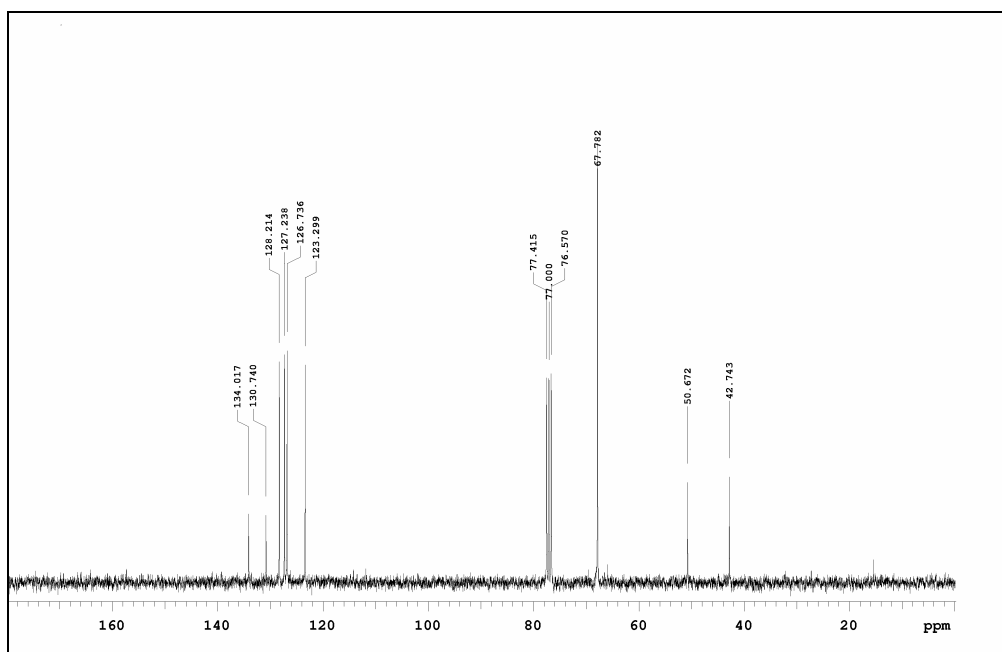
¹H-¹³C-HMBC J= 5 Hz

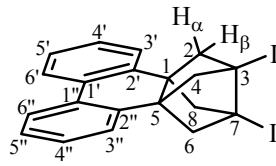


IR (KBr)

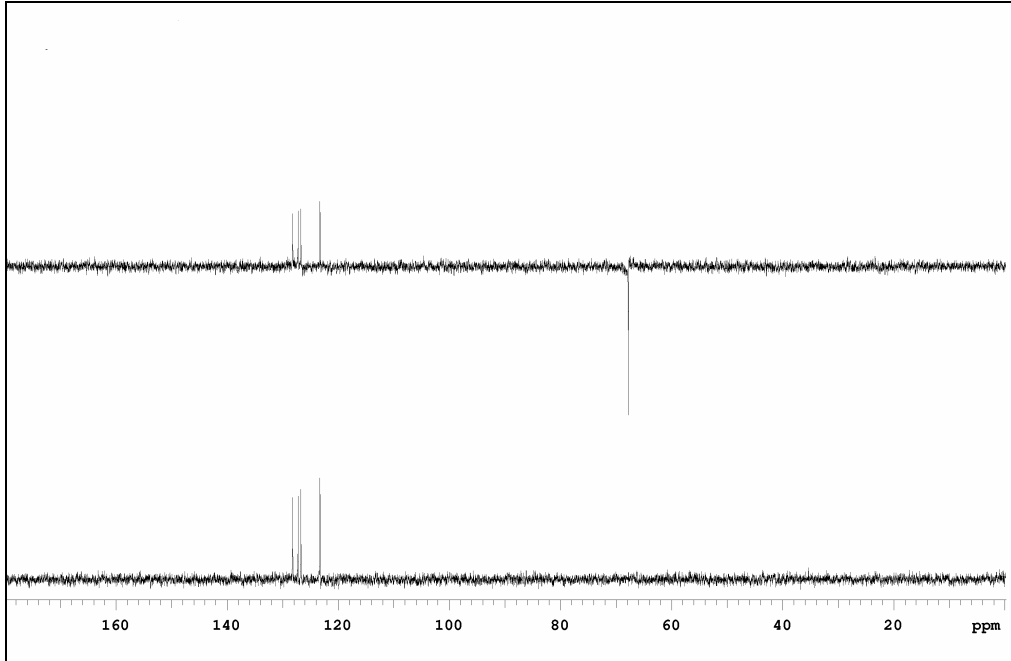


76

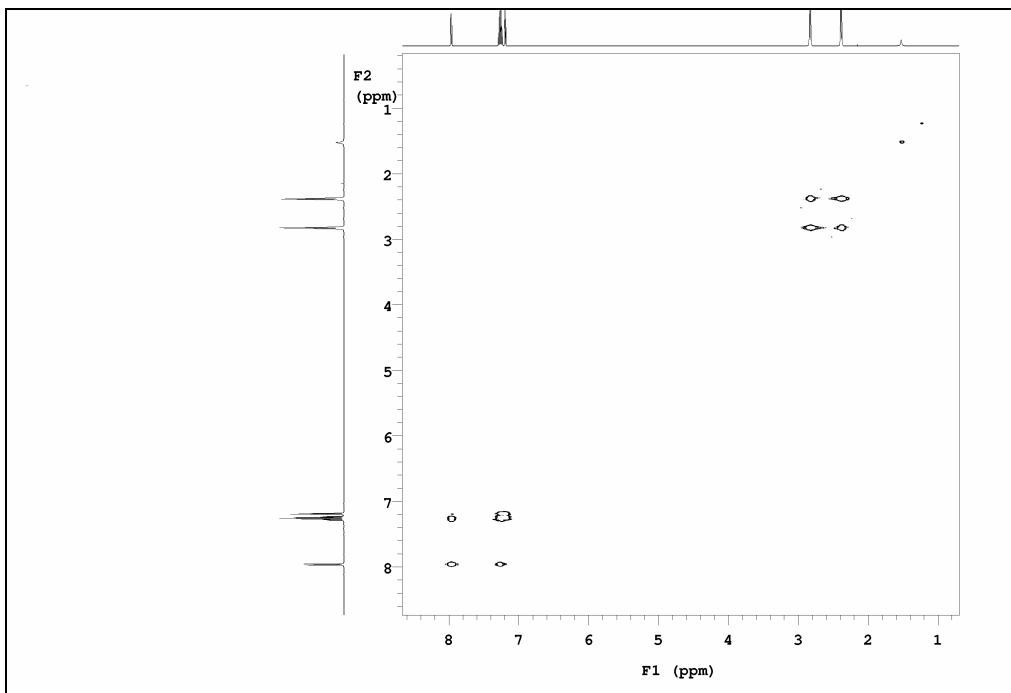
 $^1\text{H-RMN}$ (500 MHz, CDCl_3) $^{13}\text{C-RMN}$ (75.4 MHz, CDCl_3)



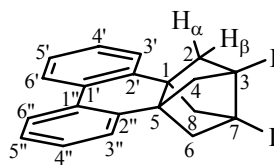
76



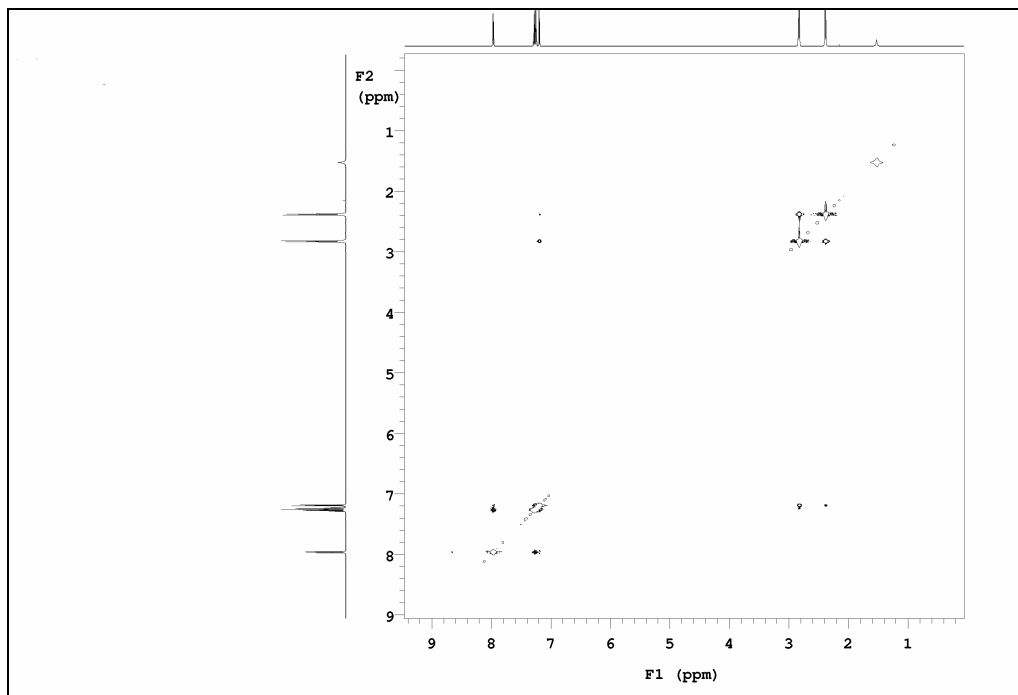
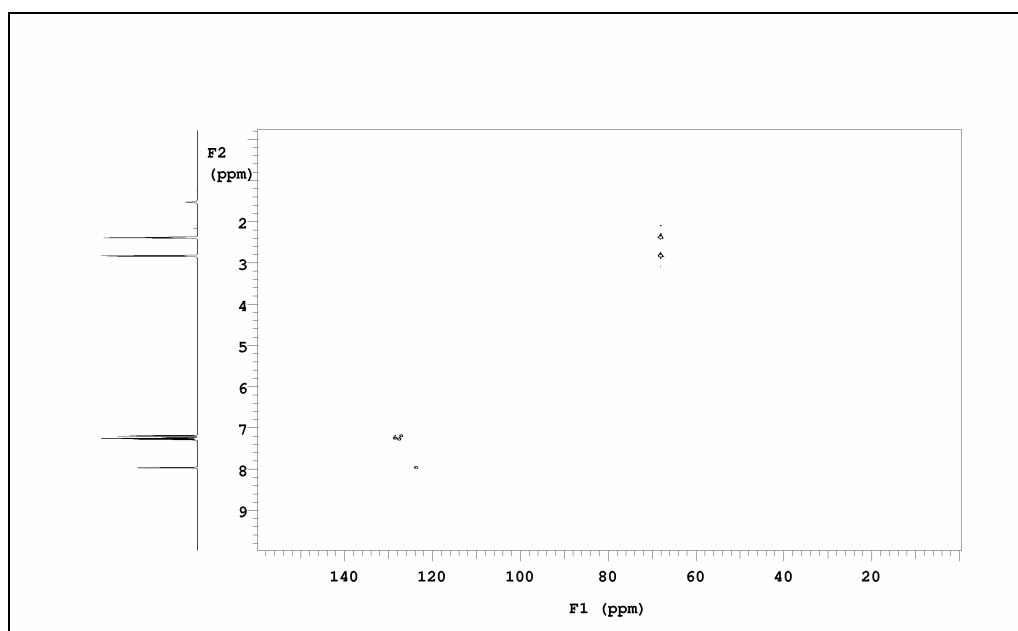
¹³C-DEPT

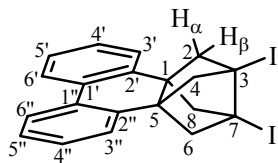


¹H-¹H-COSY

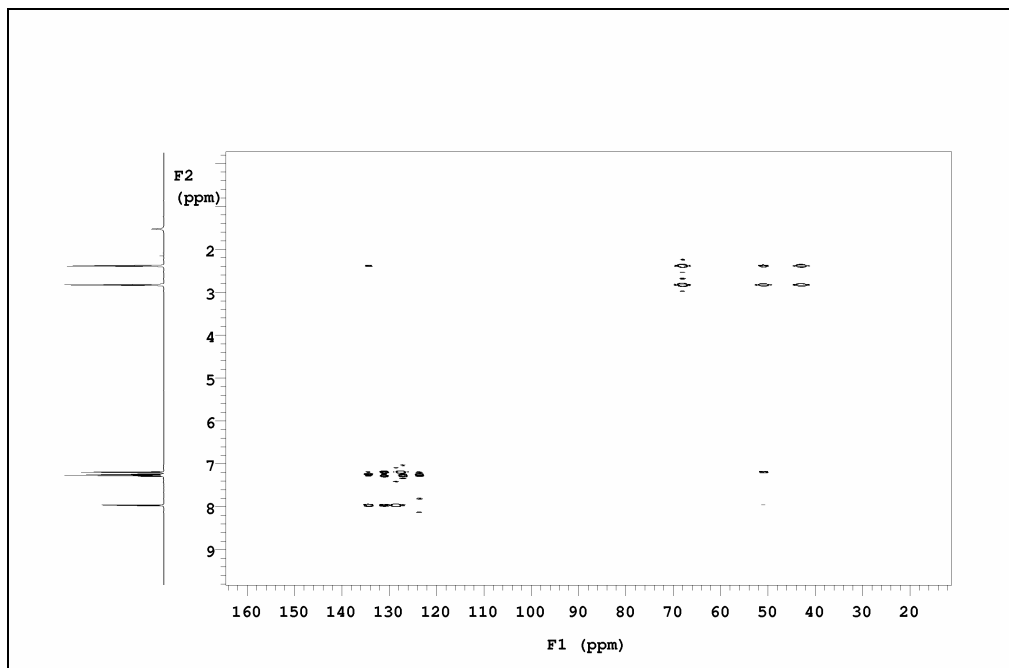


76

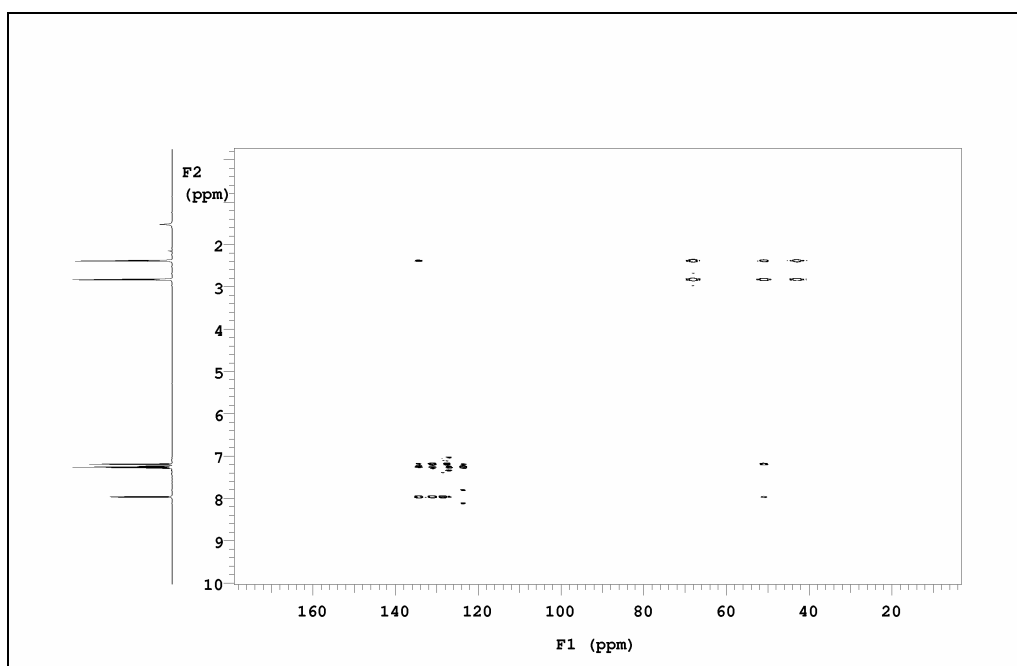
 ^1H - ^1H -NOESY ^1H - ^{13}C -HSQC



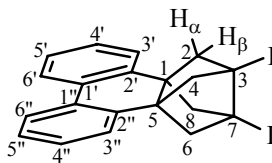
76



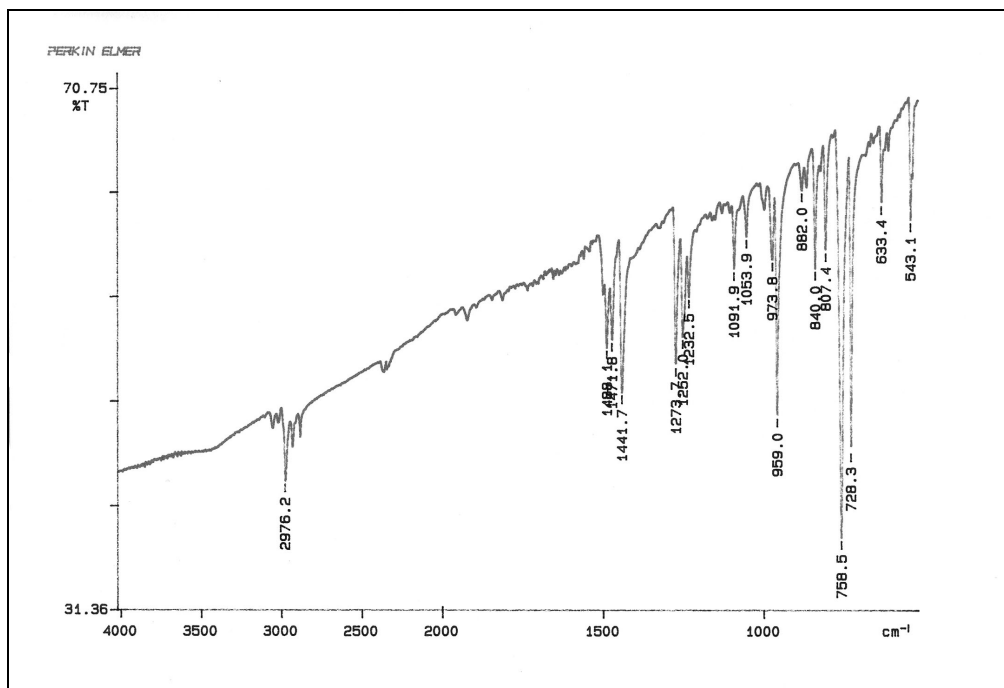
^1H - ^{13}C -HMBC $J = 8$ Hz



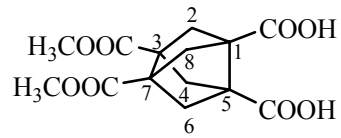
^1H - ^{13}C -HMBC $J = 5$ Hz



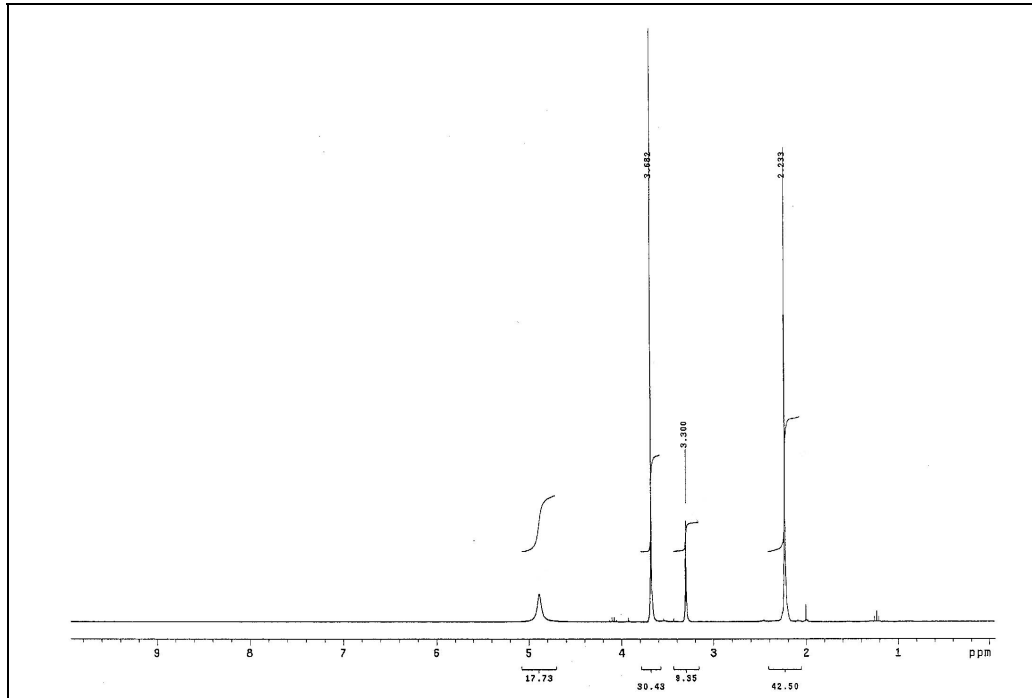
76



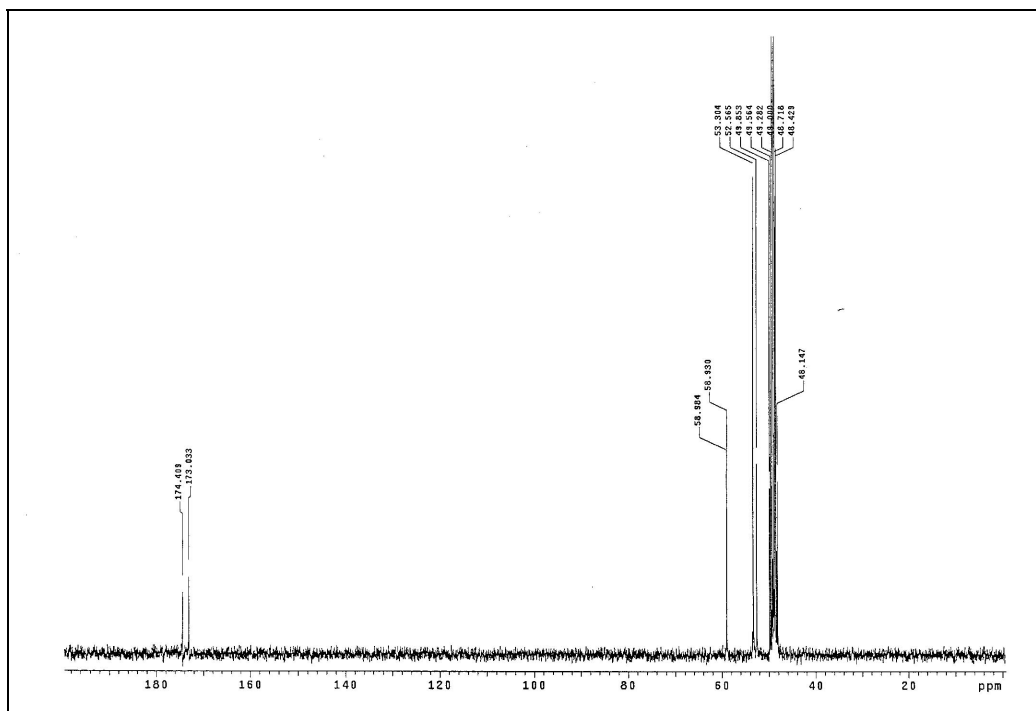
IR (KBr)



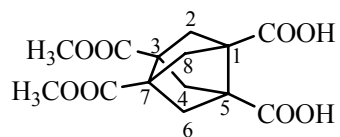
127



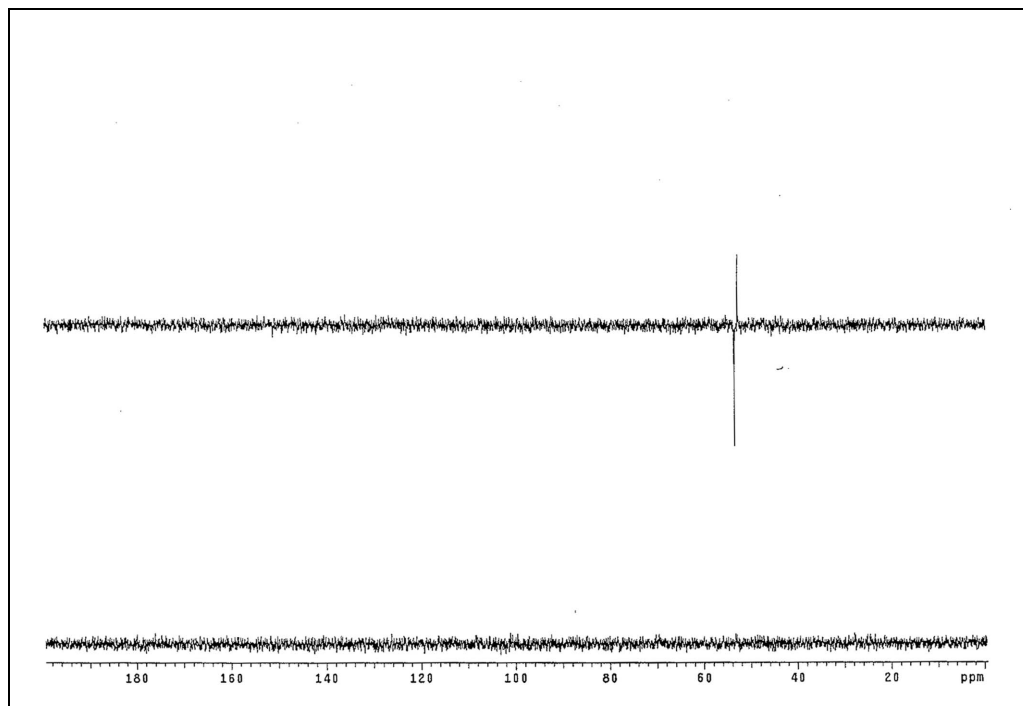
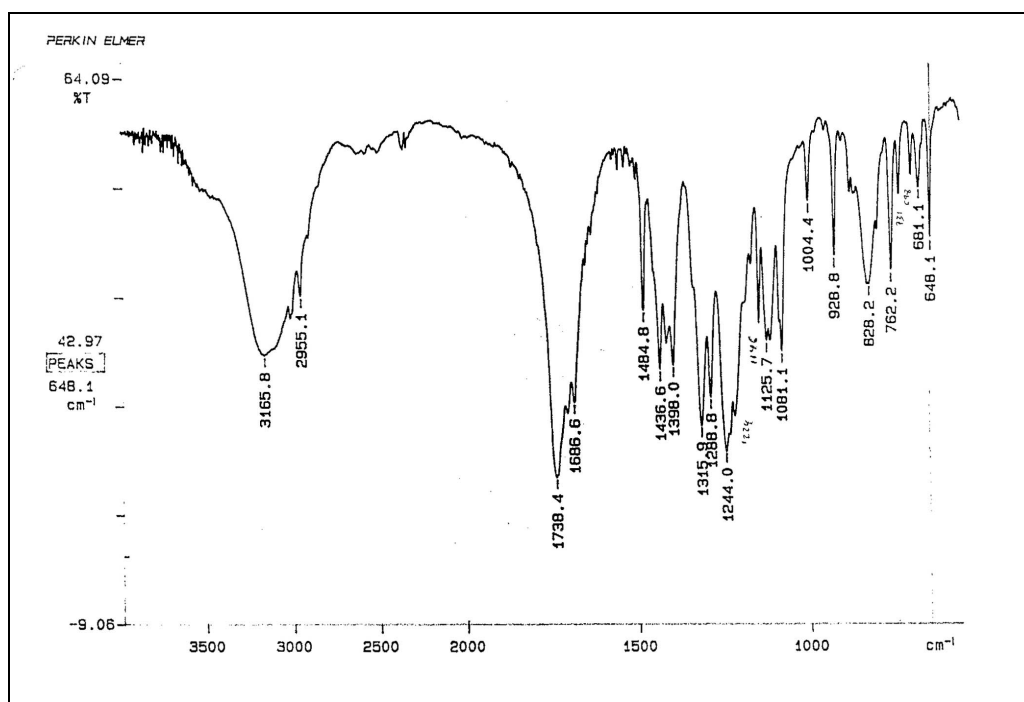
^1H -RMN (300 MHz, CD_3OD)



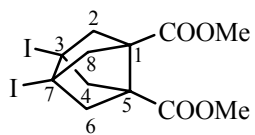
^{13}C -RMN (75.4 MHz, CD_3OD)



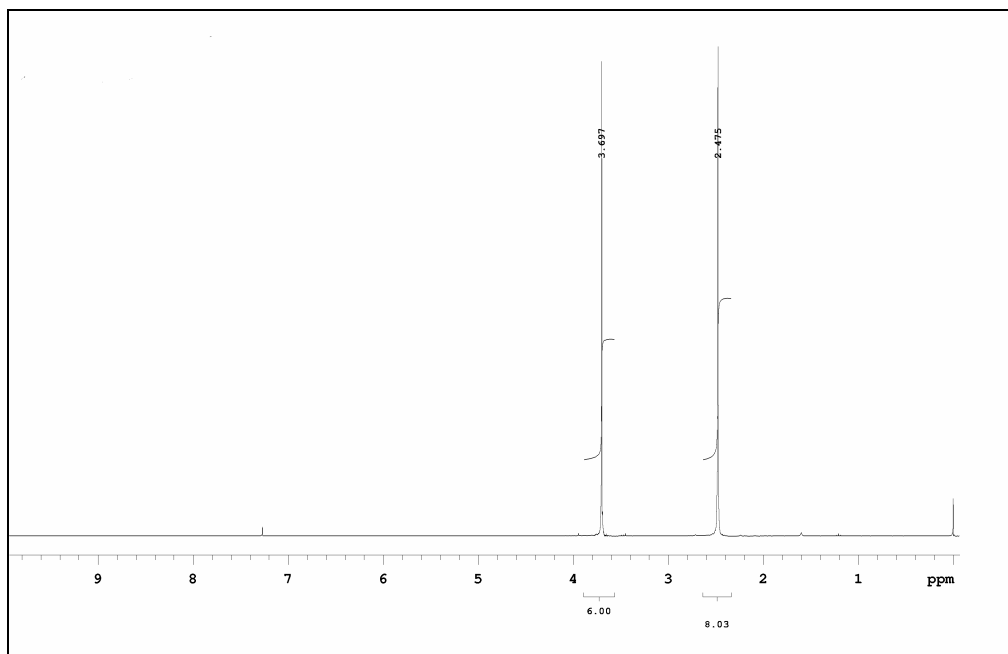
127

 ^{13}C -DEPT

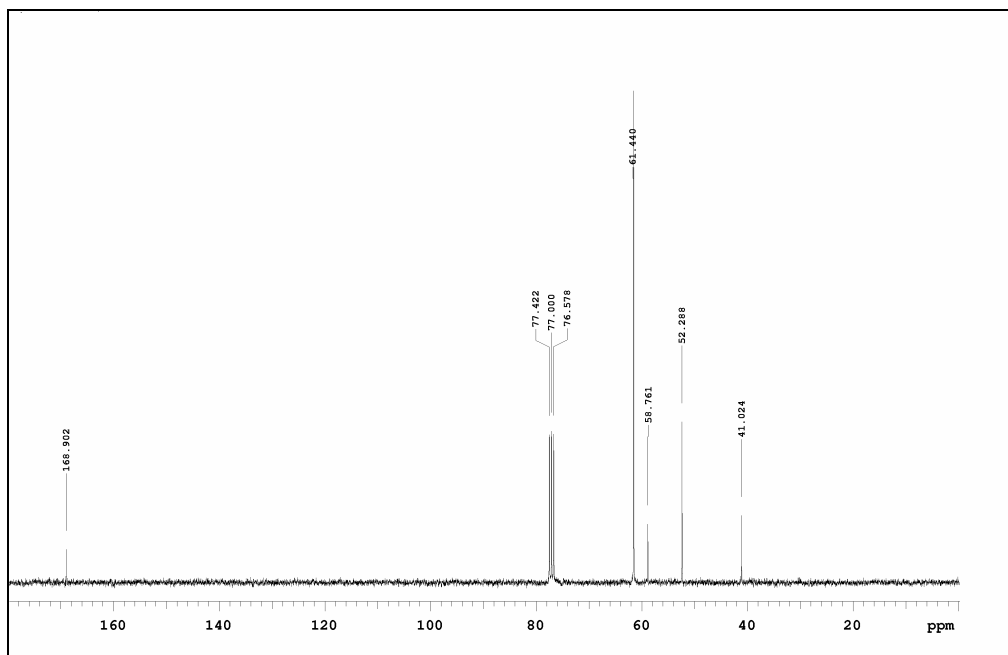
IR (KBr)



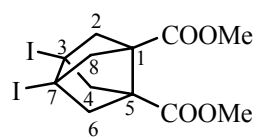
82



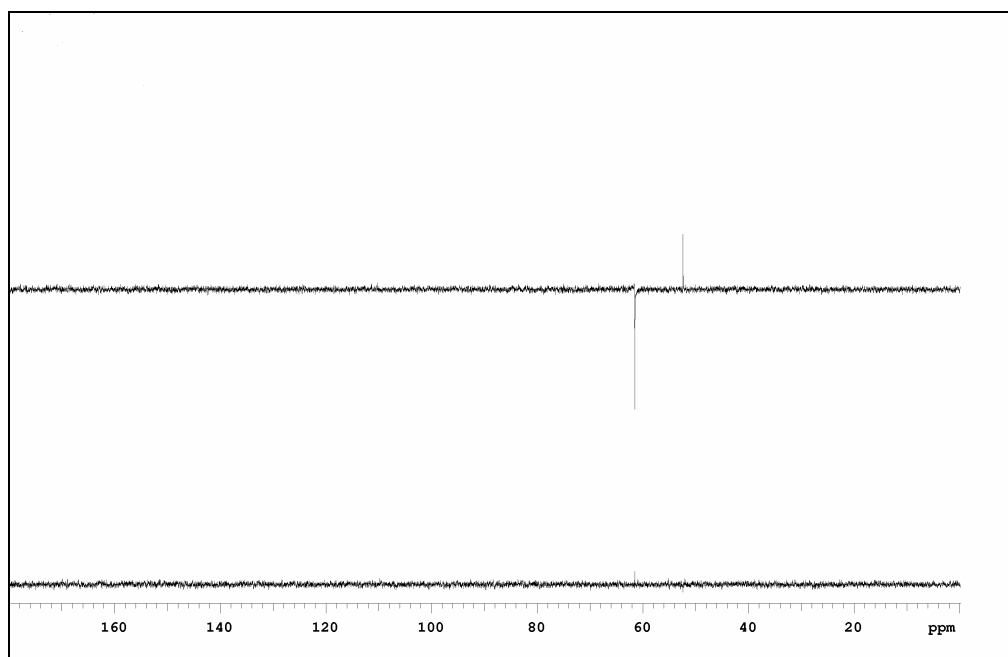
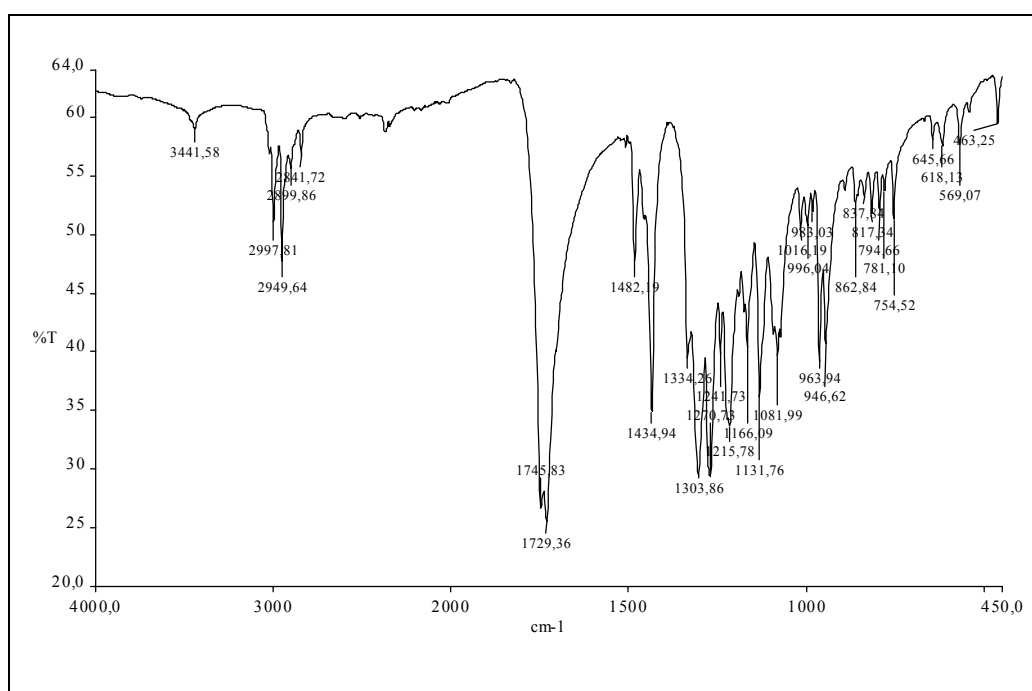
^1H -RMN (300 MHz, CDCl_3)



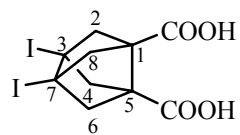
^{13}C -RMN (75.4 MHz, CDCl_3)



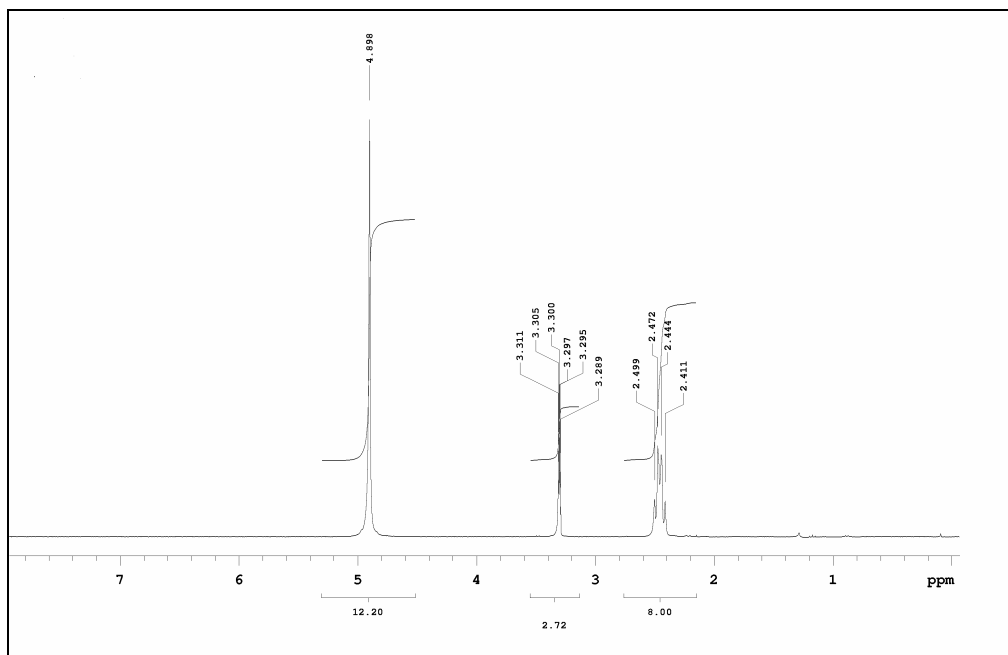
82

 ^{13}C -DEPT

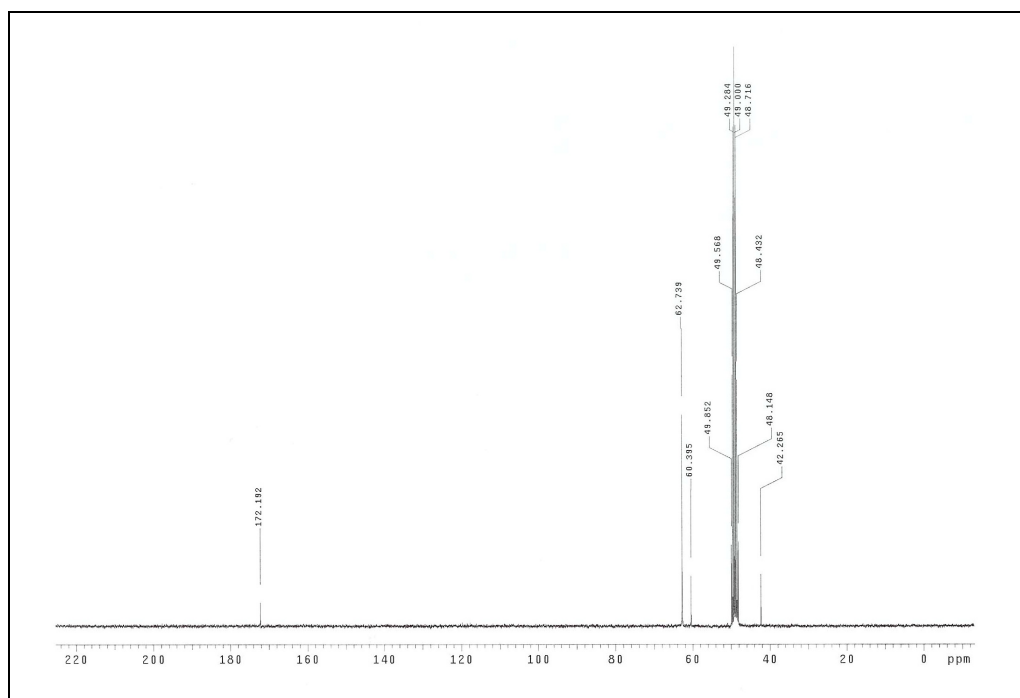
IR (KBr)



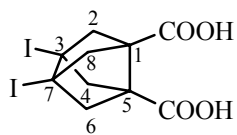
128



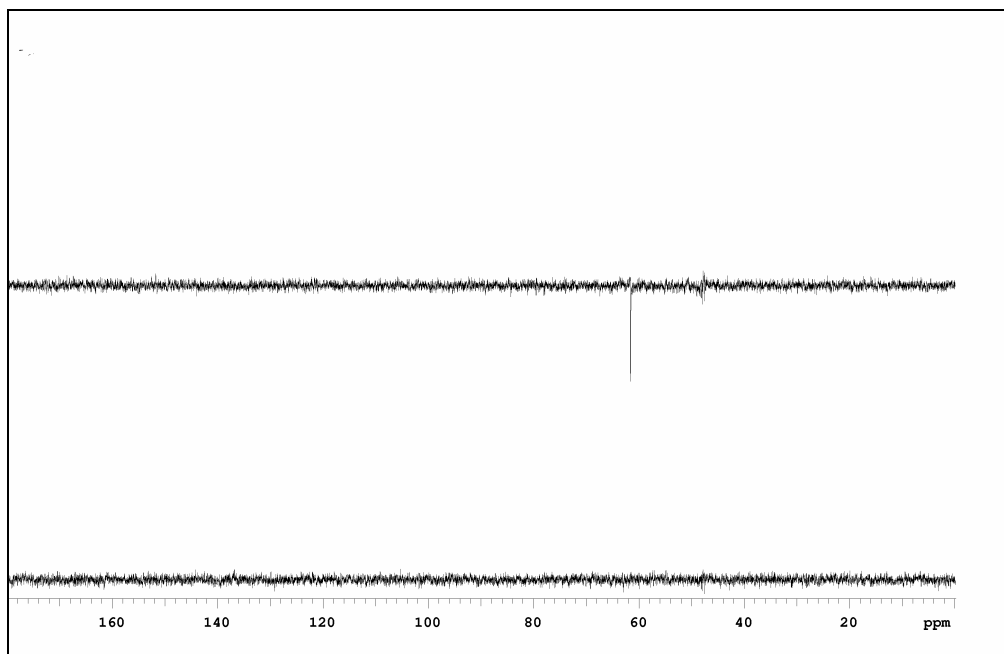
$^1\text{H-RMN}$ (300 MHz, CD_3OD)



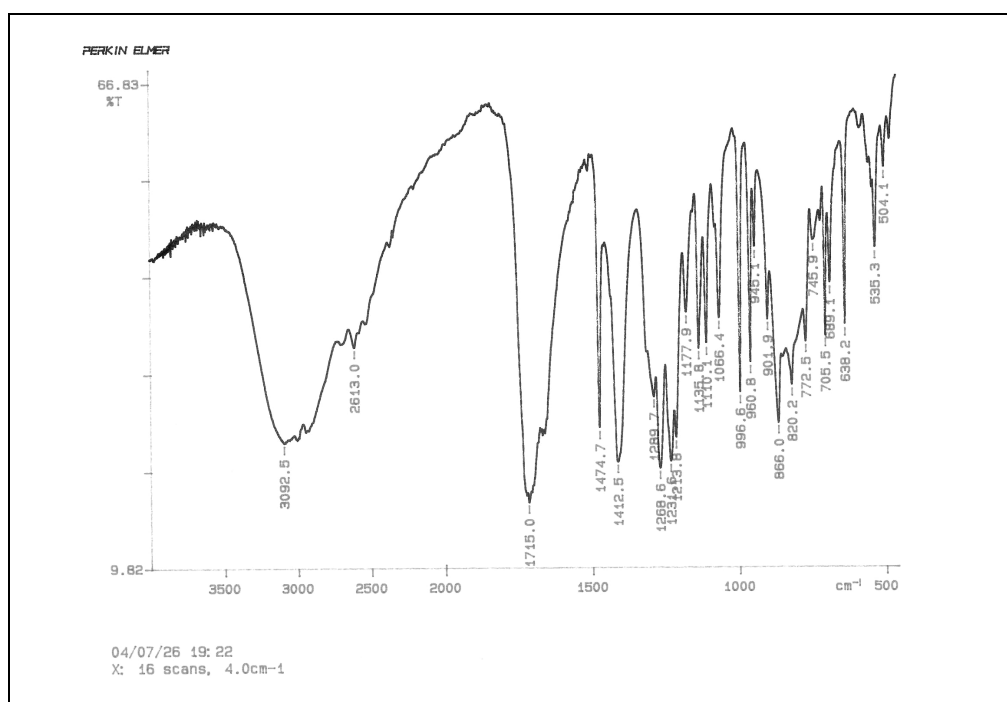
$^{13}\text{C-RMN}$ (75.4 MHz, CD_3OD)



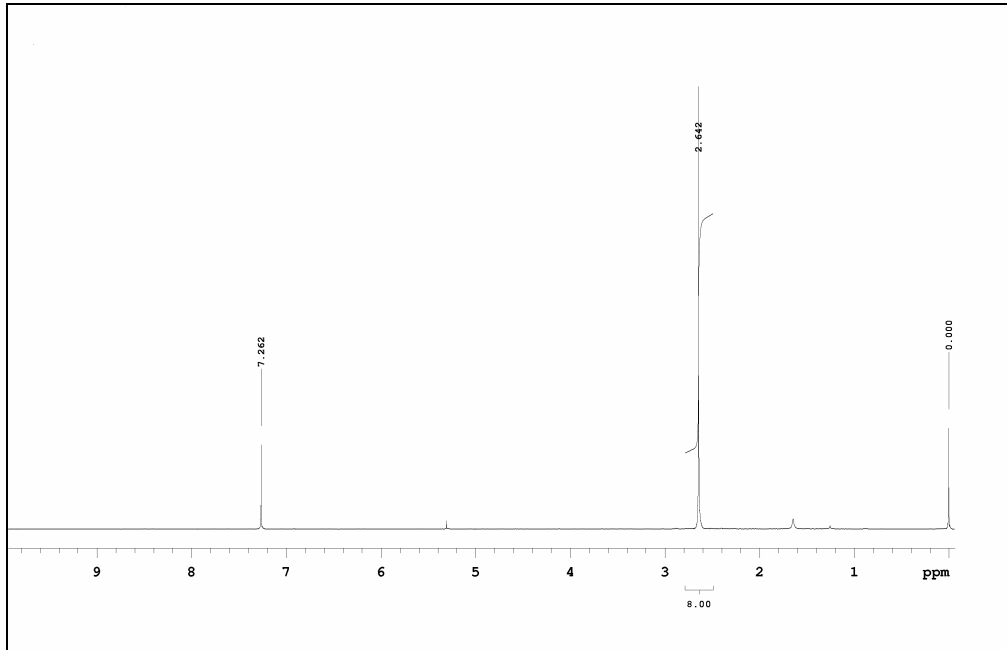
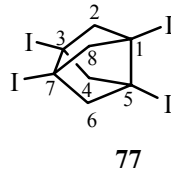
128



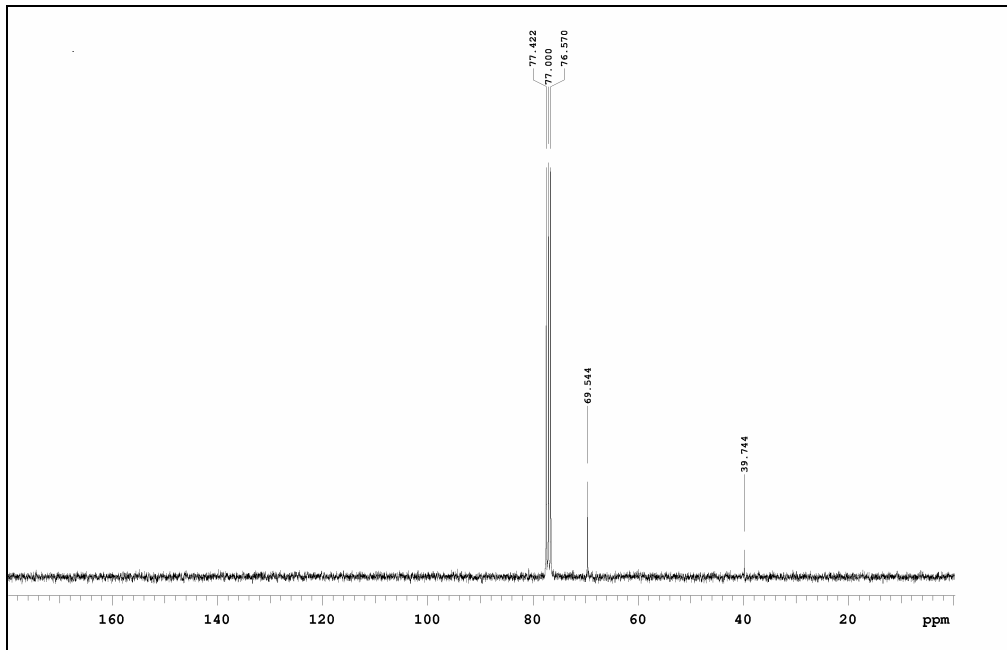
¹³C-DEPT



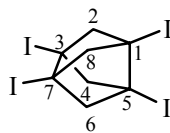
IR (KBr)



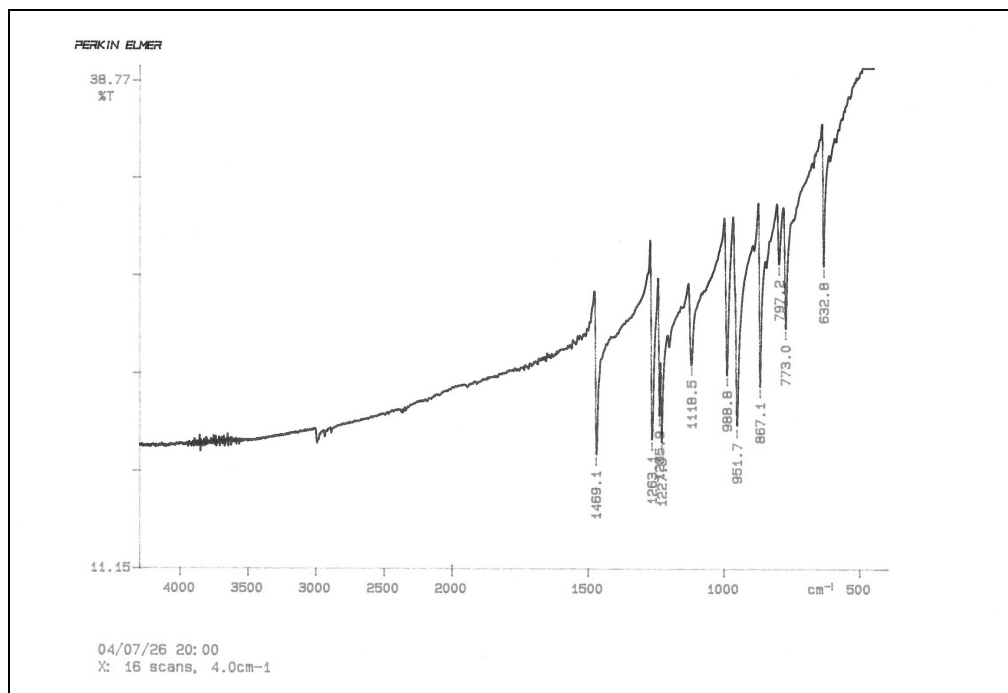
^1H -RMN (300 MHz, CDCl_3)



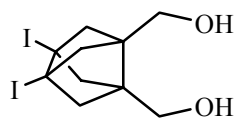
^{13}C -RMN (75.4 MHz, CDCl_3)



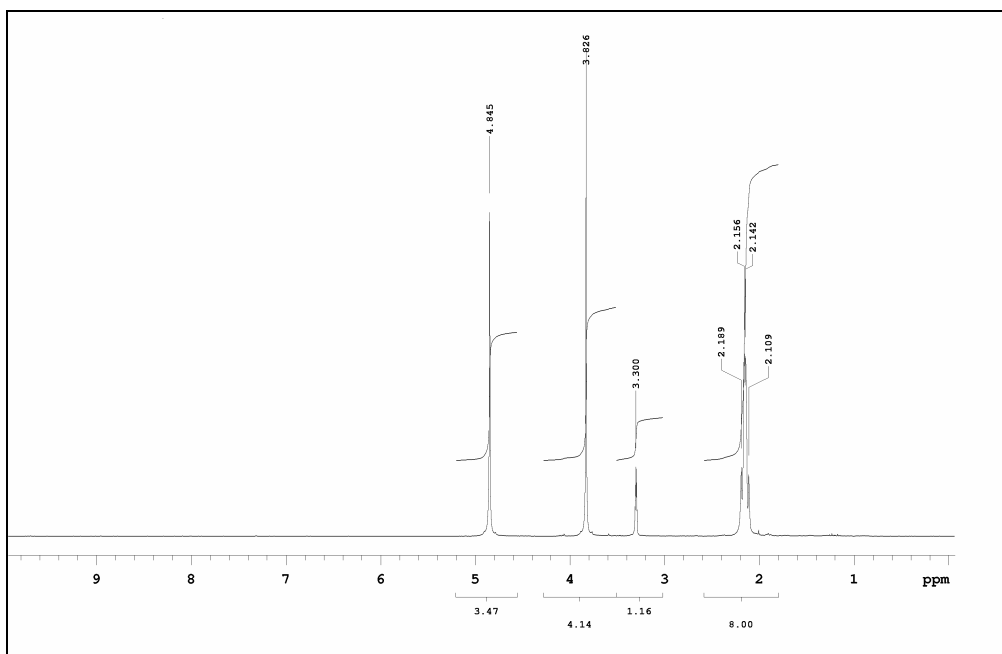
77



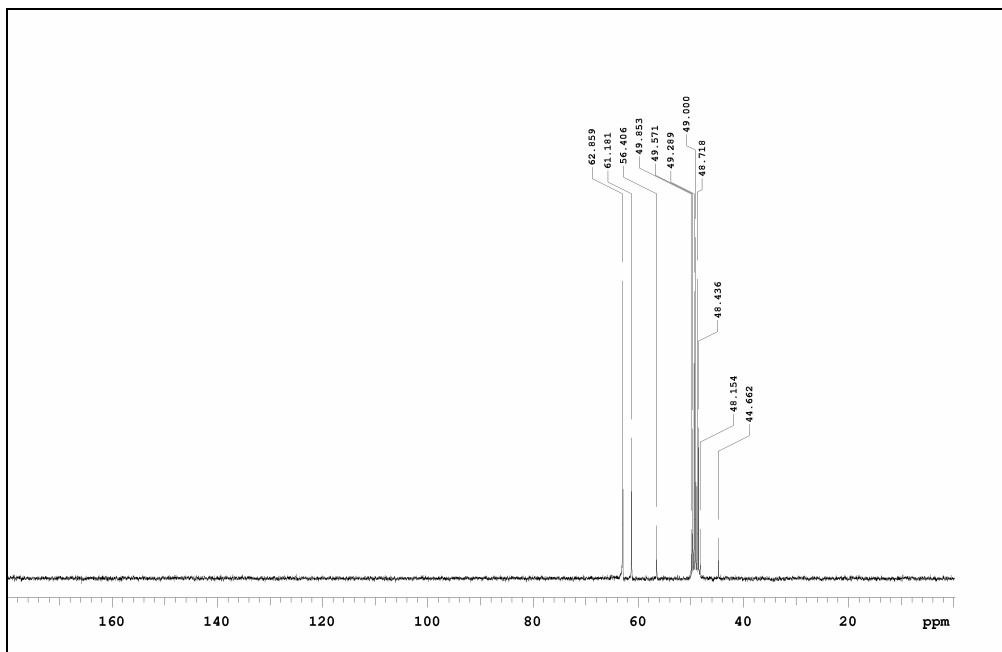
IR (KBr)



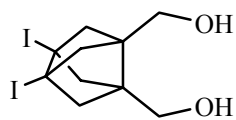
141



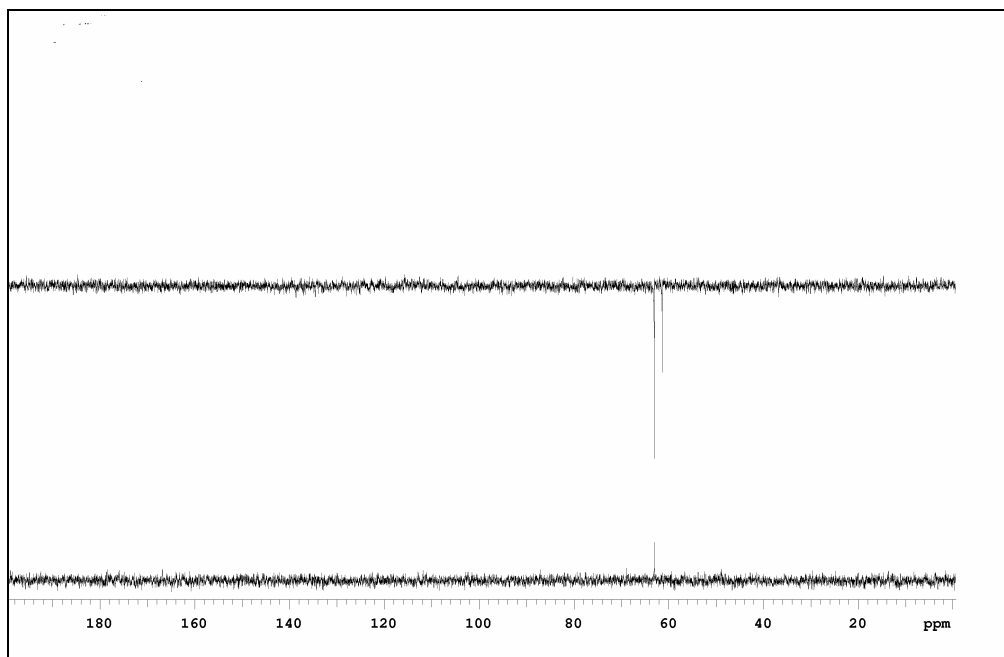
^1H -RMN (300 MHz, CD_3OD)



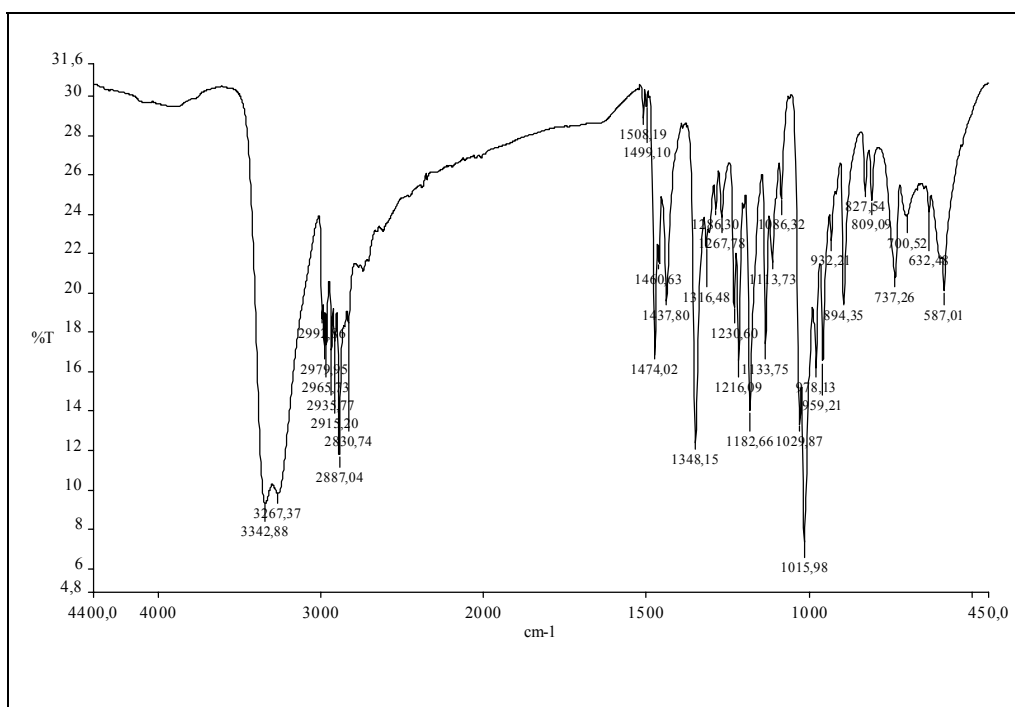
^{13}C -RMN (75.4 MHz, CD_3OD)



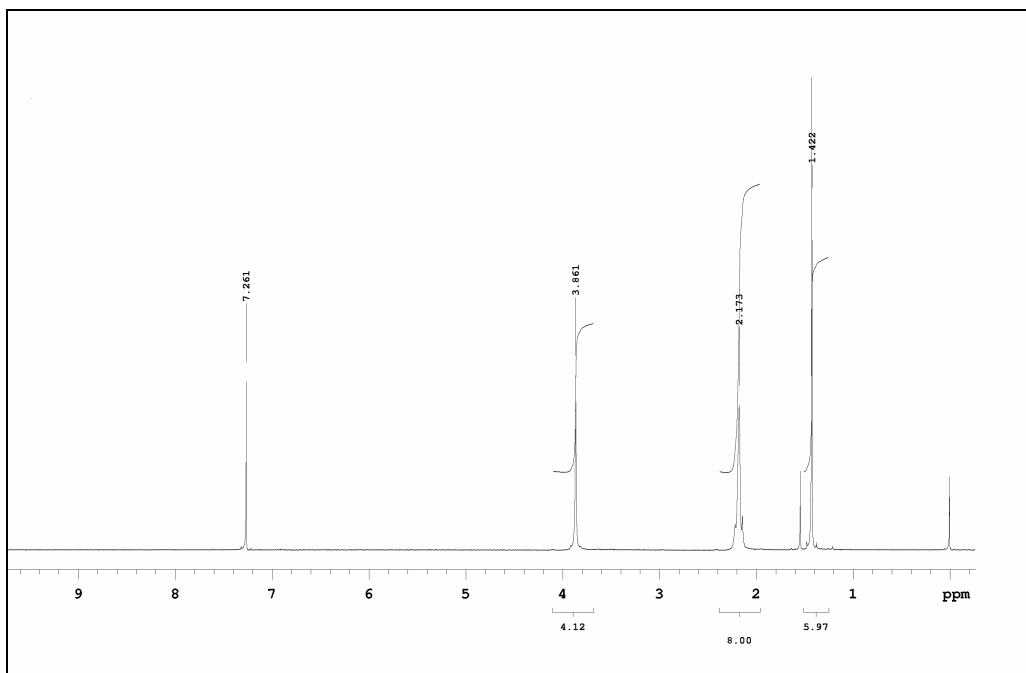
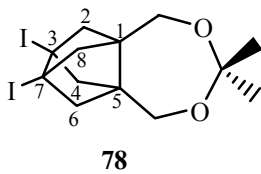
141



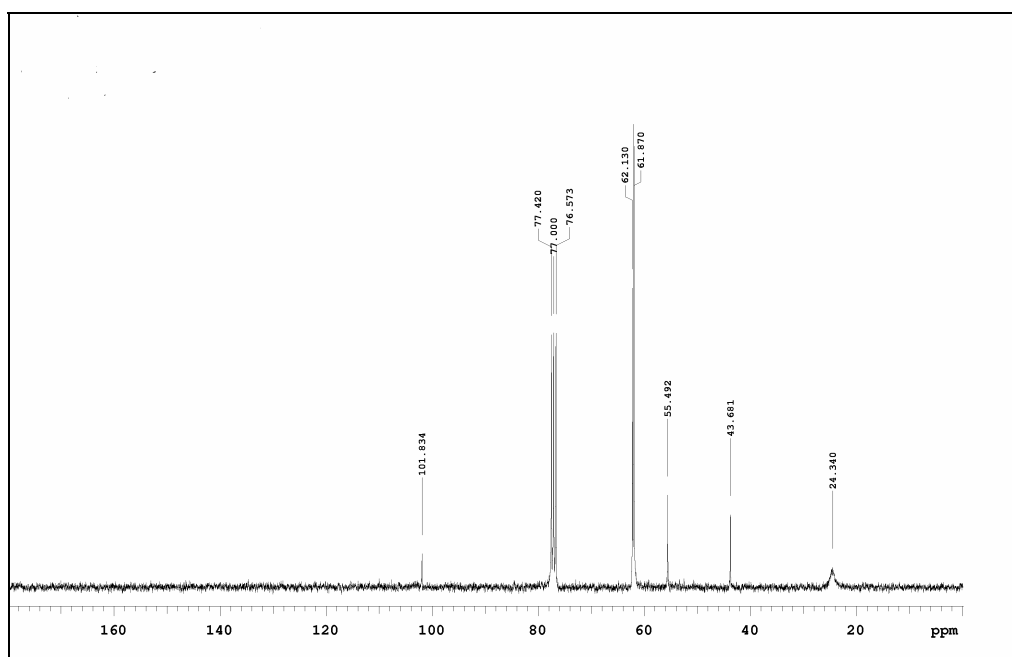
^{13}C -DEPT



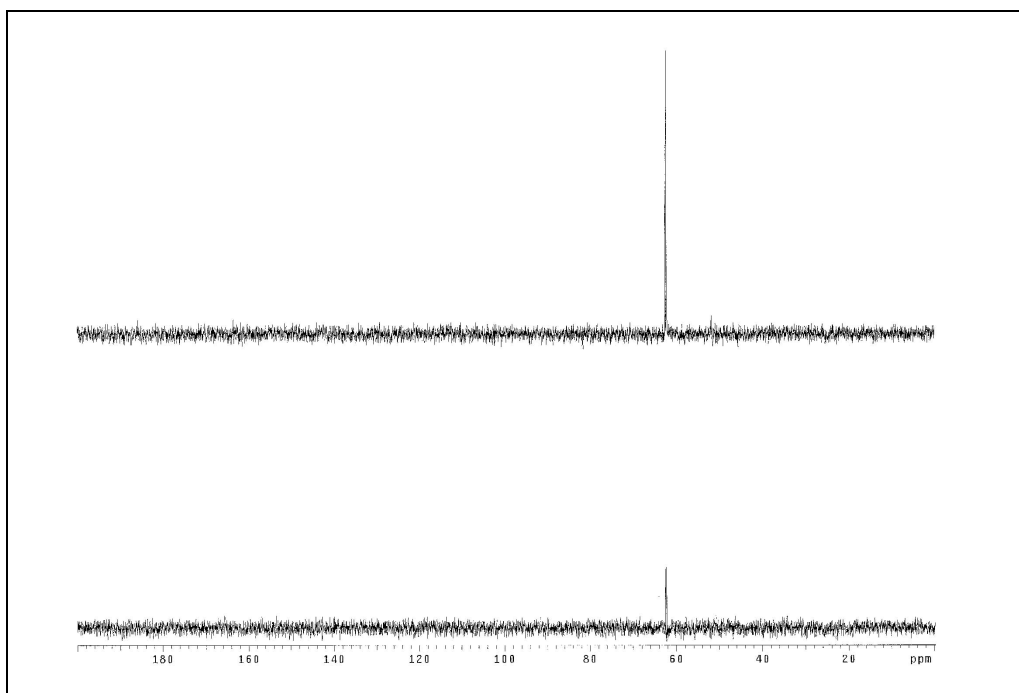
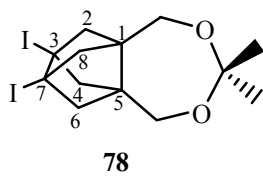
IR (KBr)



^1H -RMN (300 MHz, CDCl_3)

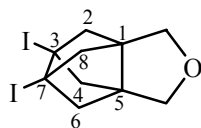


^{13}C -RMN (75.4 MHz, CDCl_3)

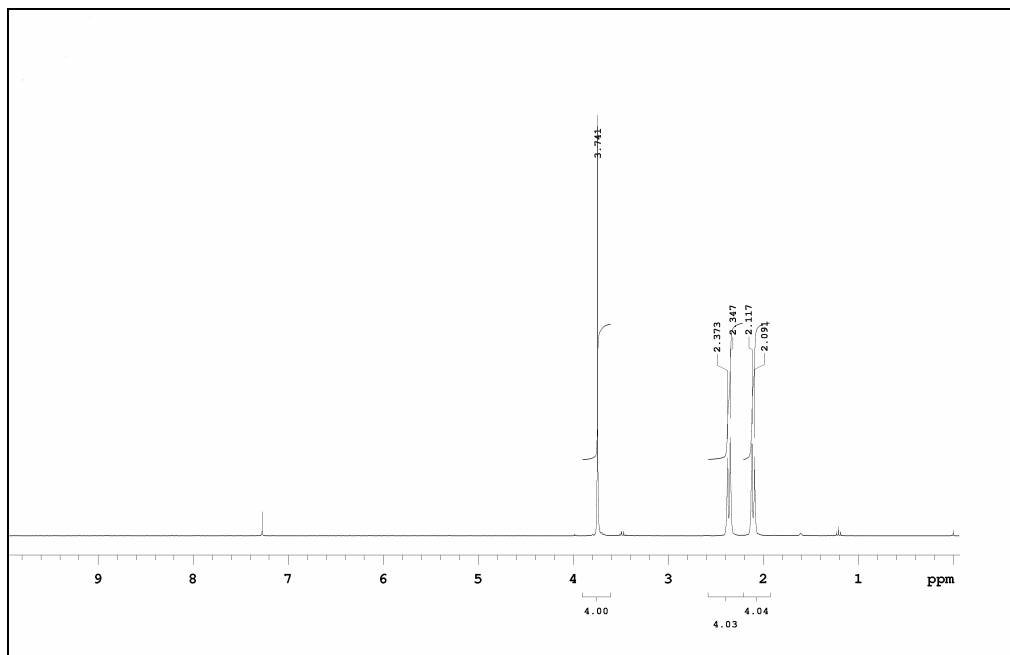


^{13}C -DEPT (75.4 MHz, CDCl_3)

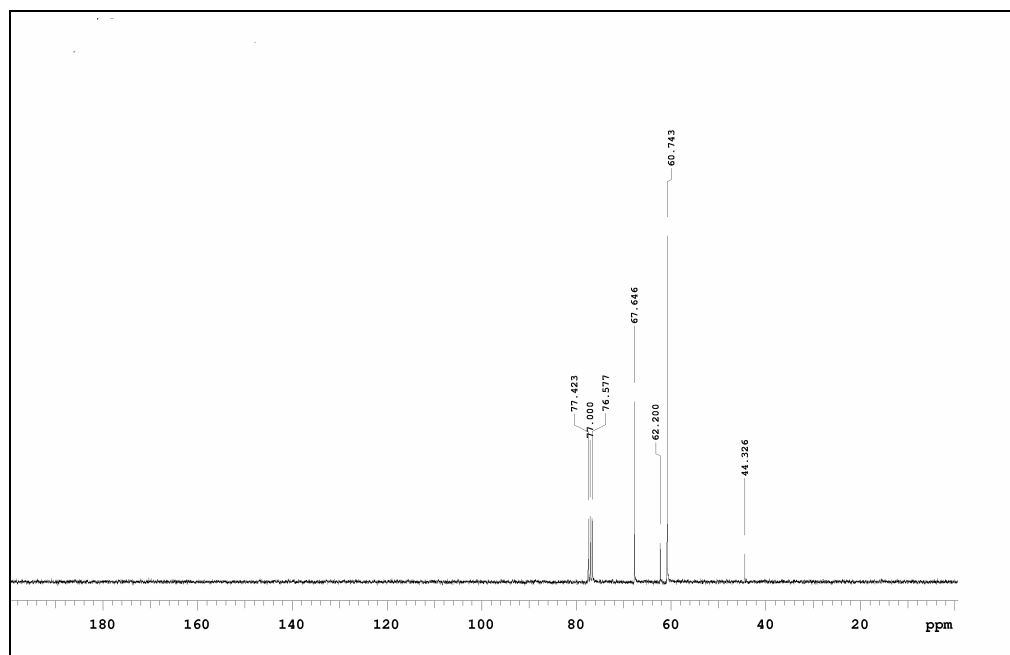
IR (KBr)



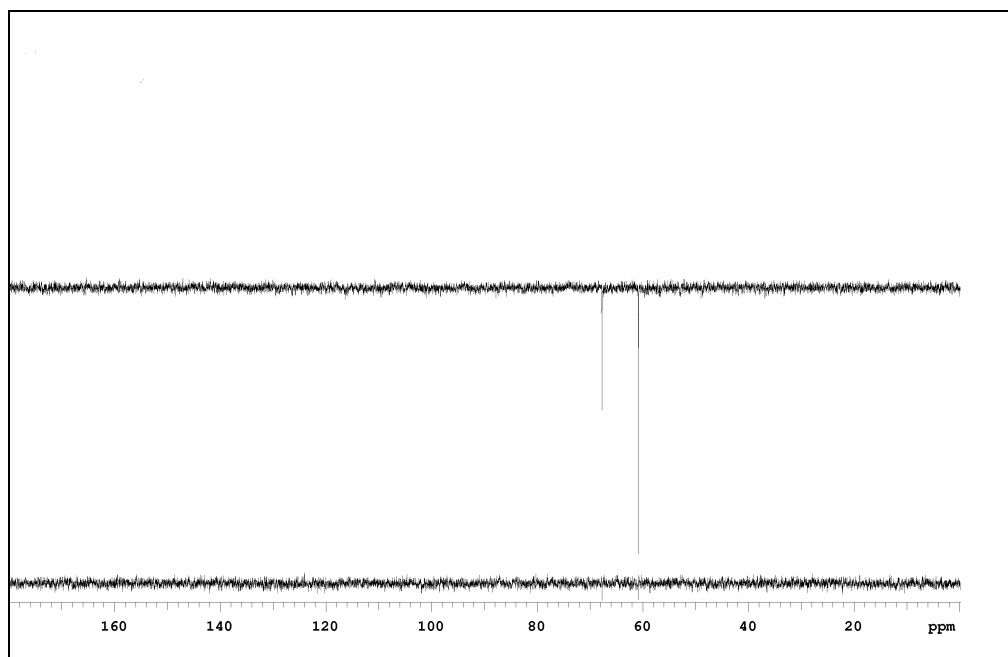
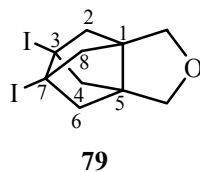
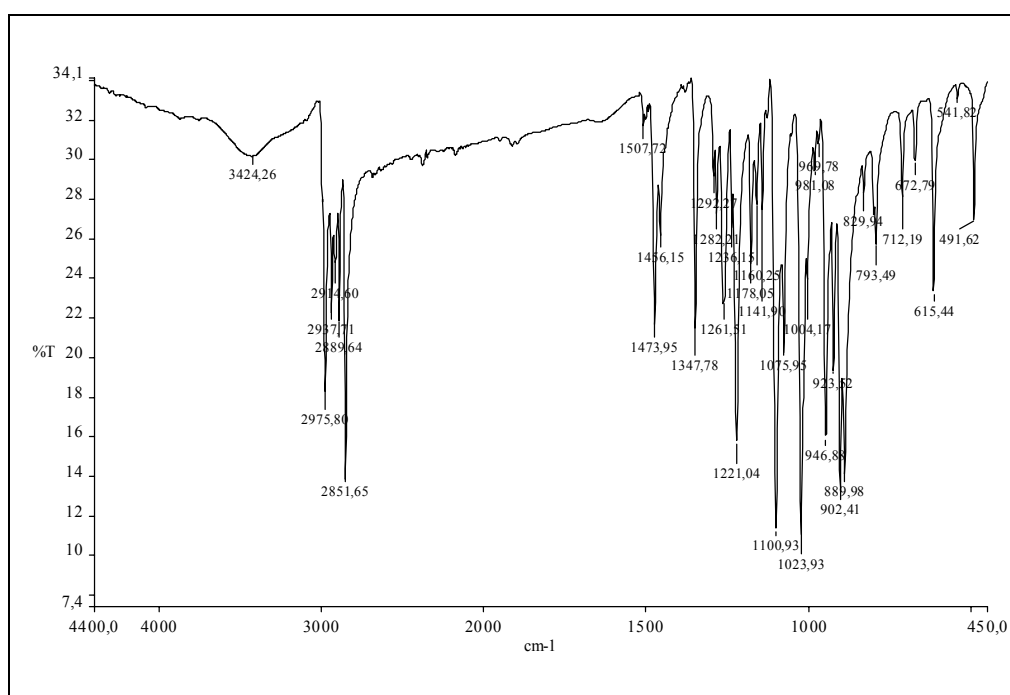
79



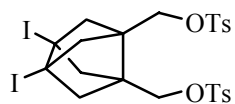
$^1\text{H-RMN}$ (300 MHz, CDCl_3)



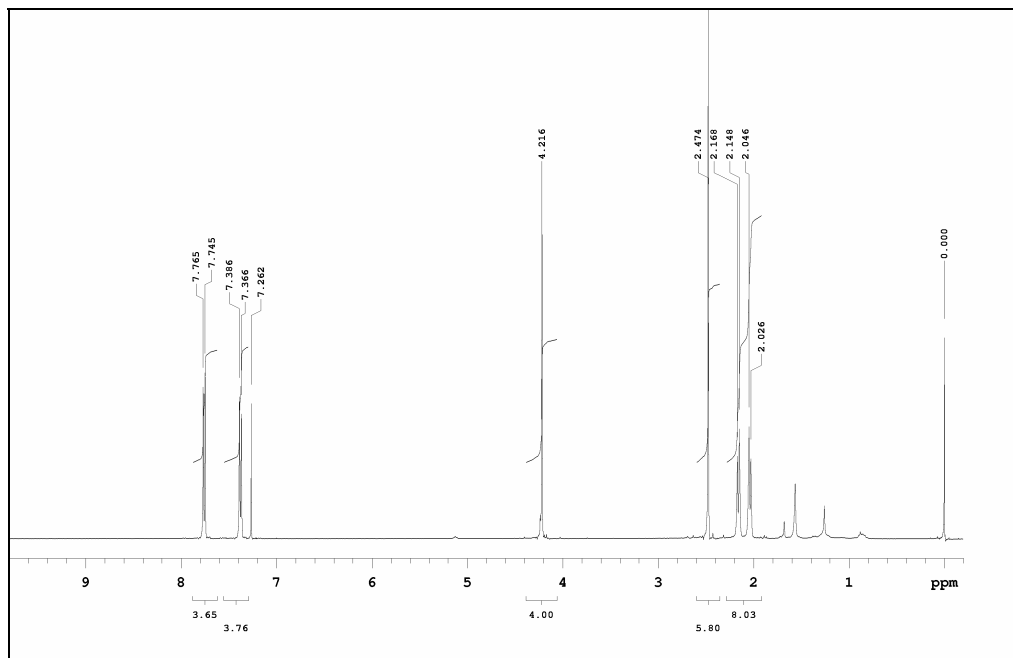
$^{13}\text{C-RMN}$ (75.4 MHz, CDCl_3)

 ^{13}C -DEPT

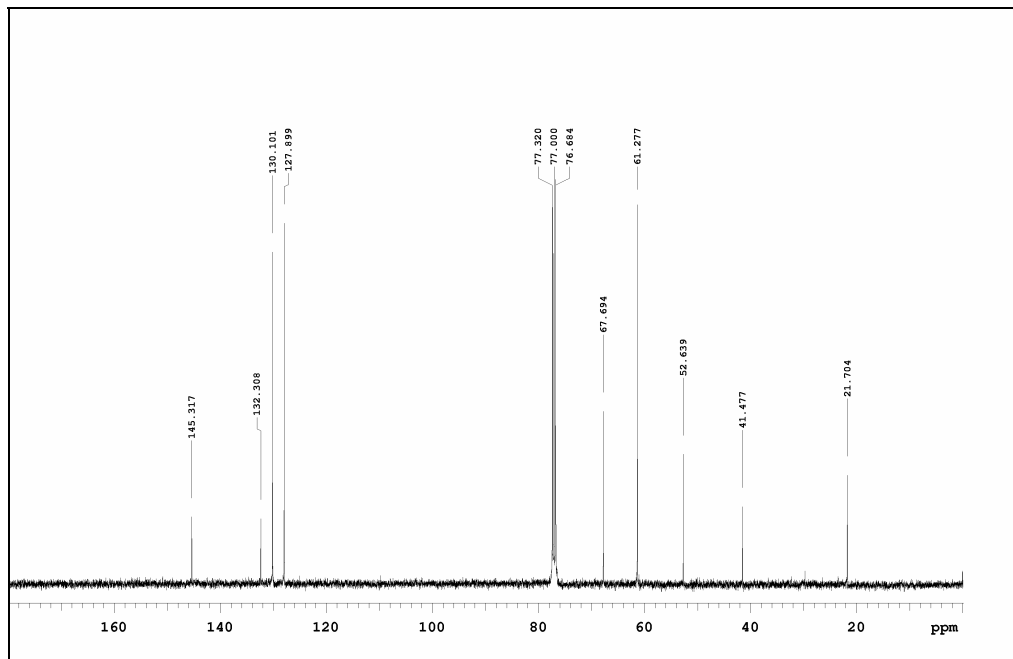
IR (KBr)



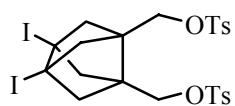
142



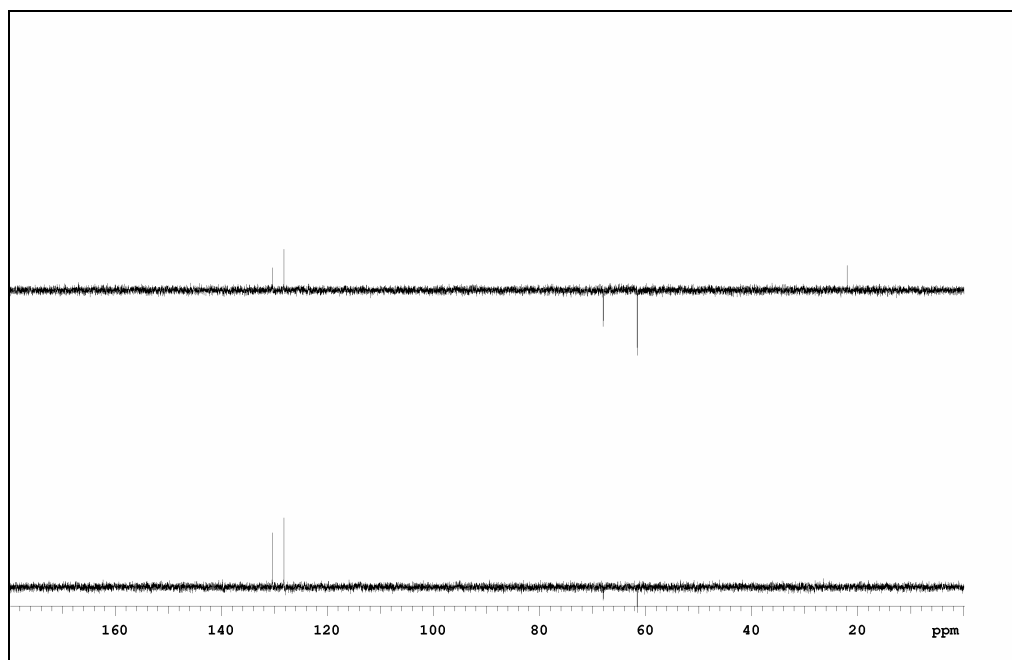
$^1\text{H-RMN}$ (400 MHz, CDCl_3)



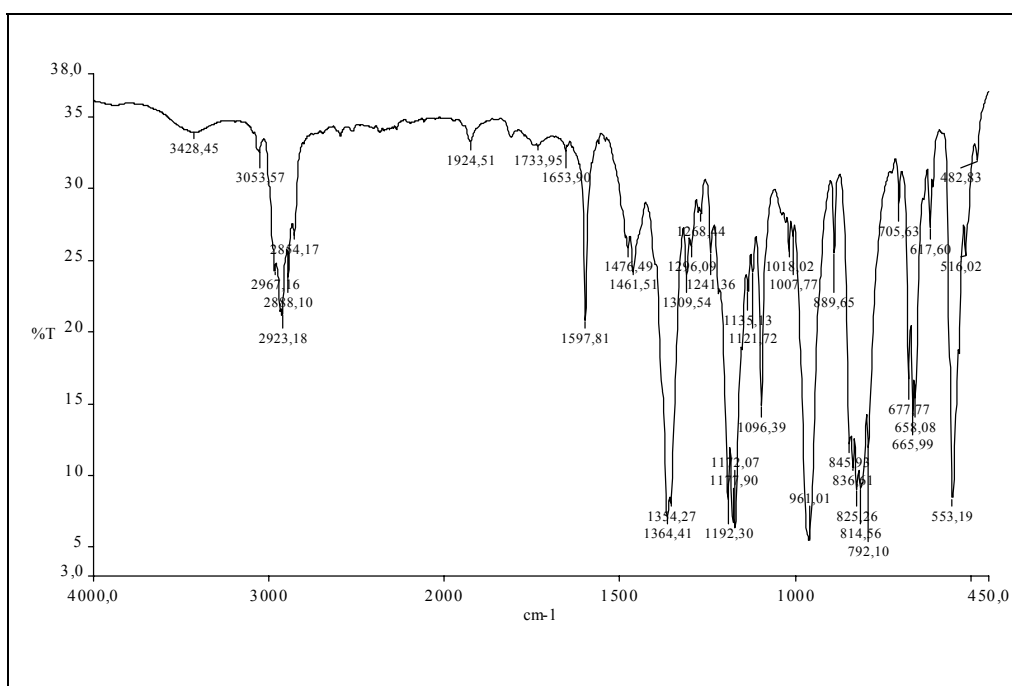
$^{13}\text{C-RMN}$ (100.6 MHz, CDCl_3)



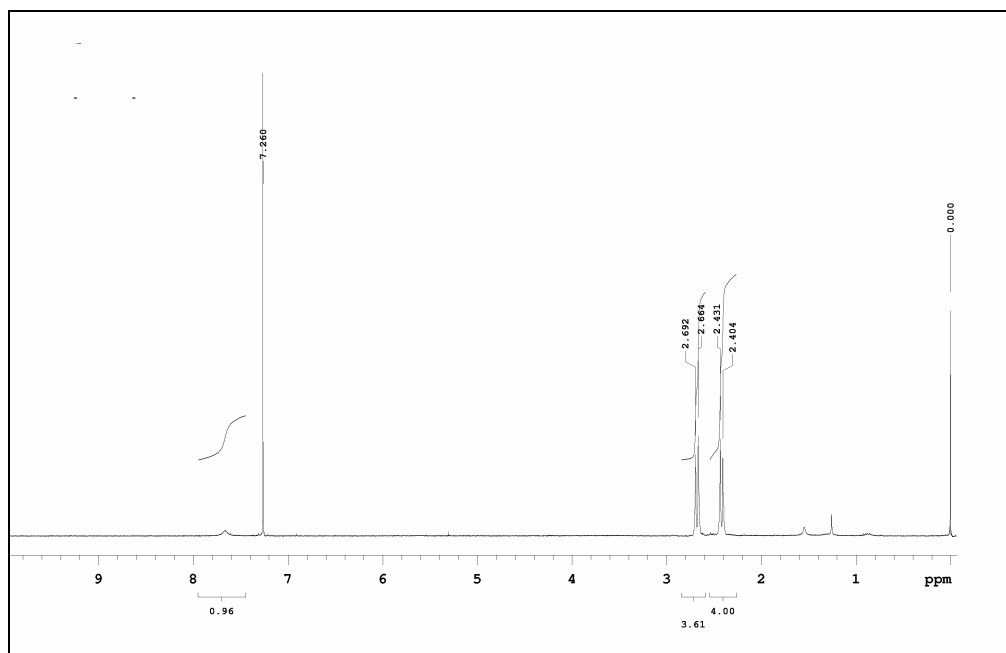
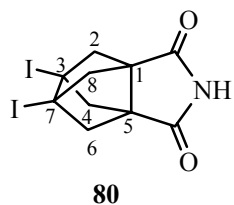
142



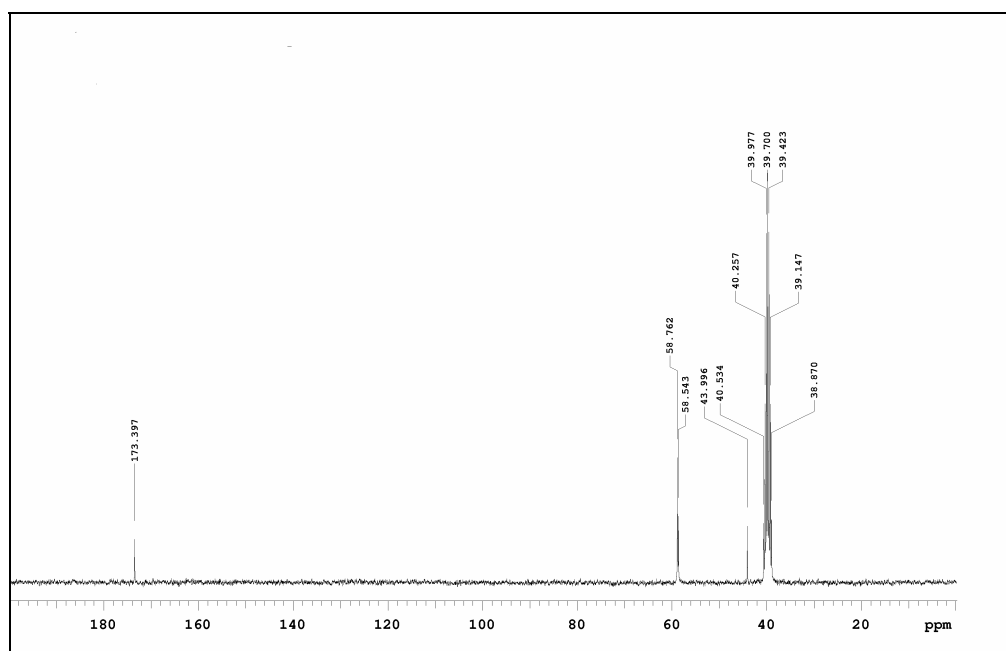
¹³C-DEPT



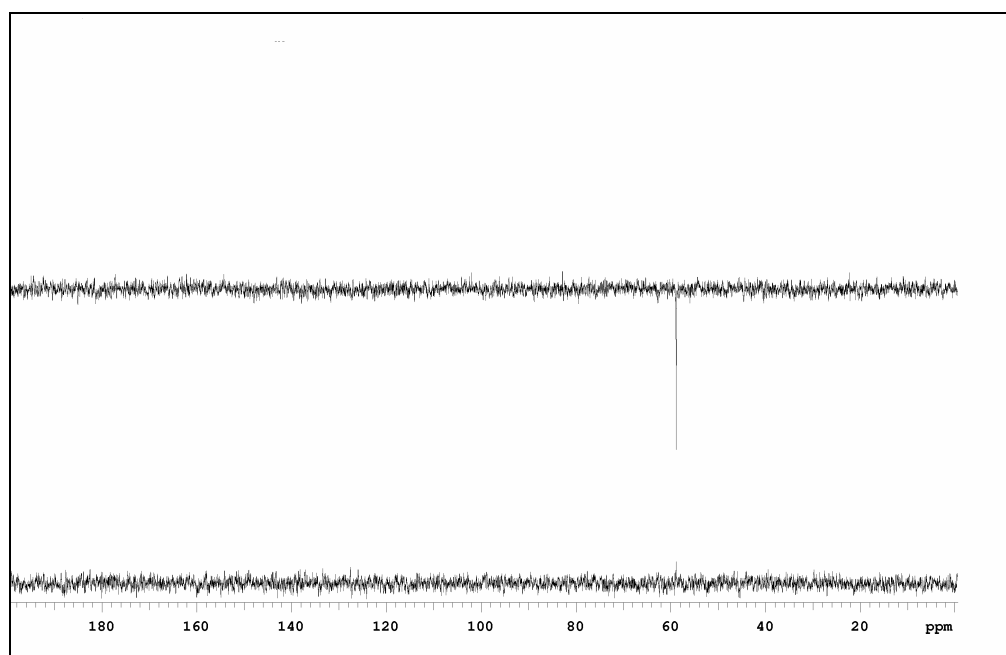
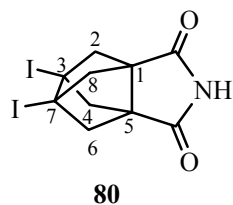
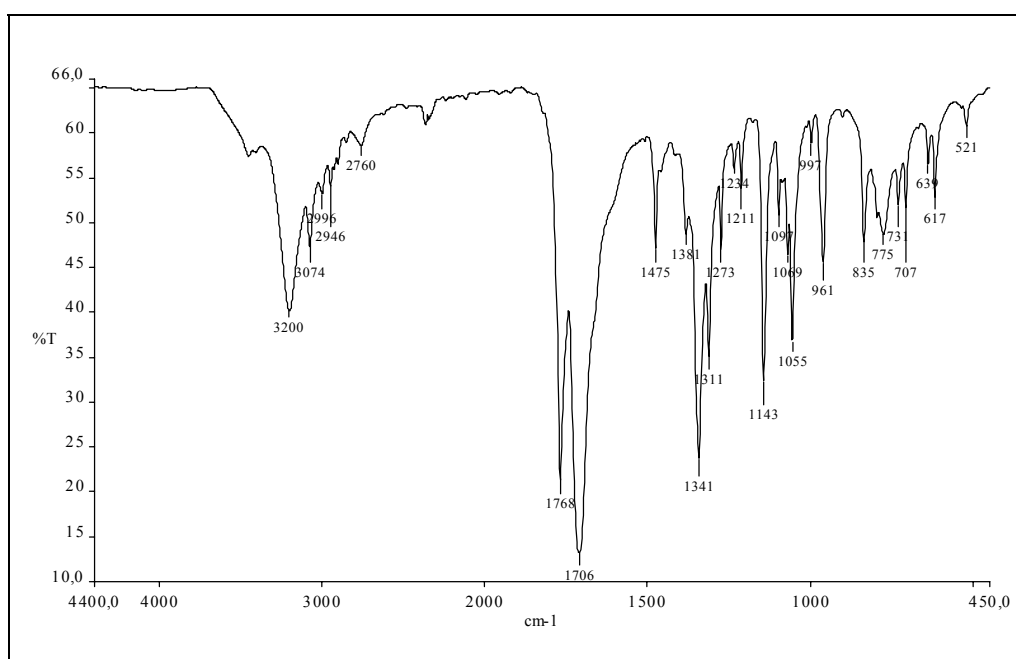
IR (KBr)



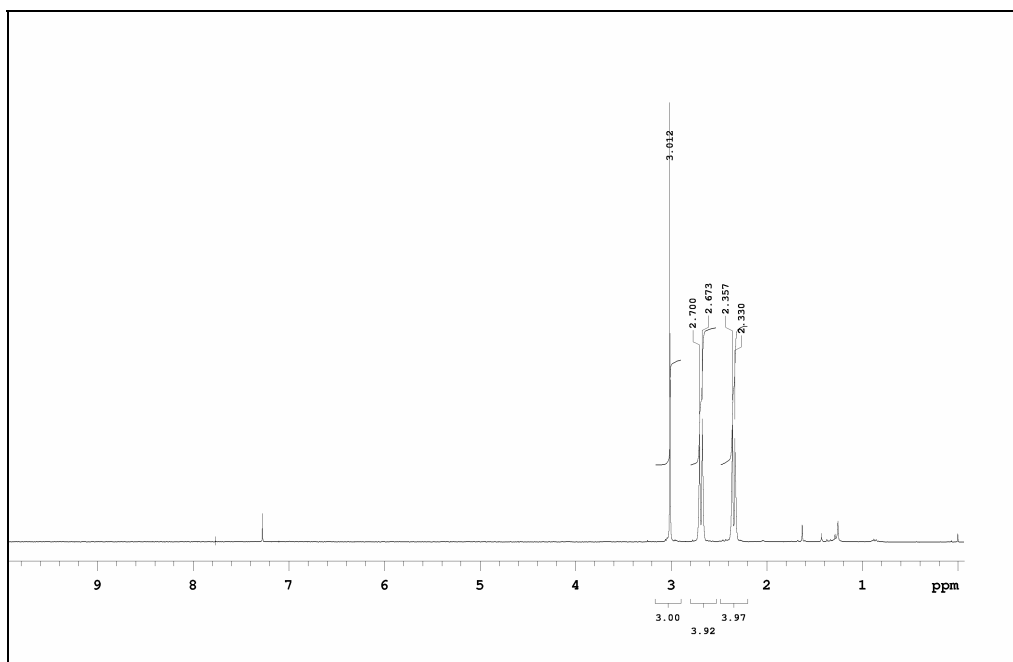
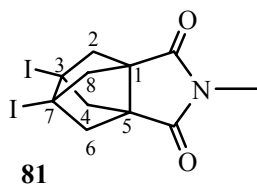
$^1\text{H-RMN}$ (300 MHz, CDCl_3)



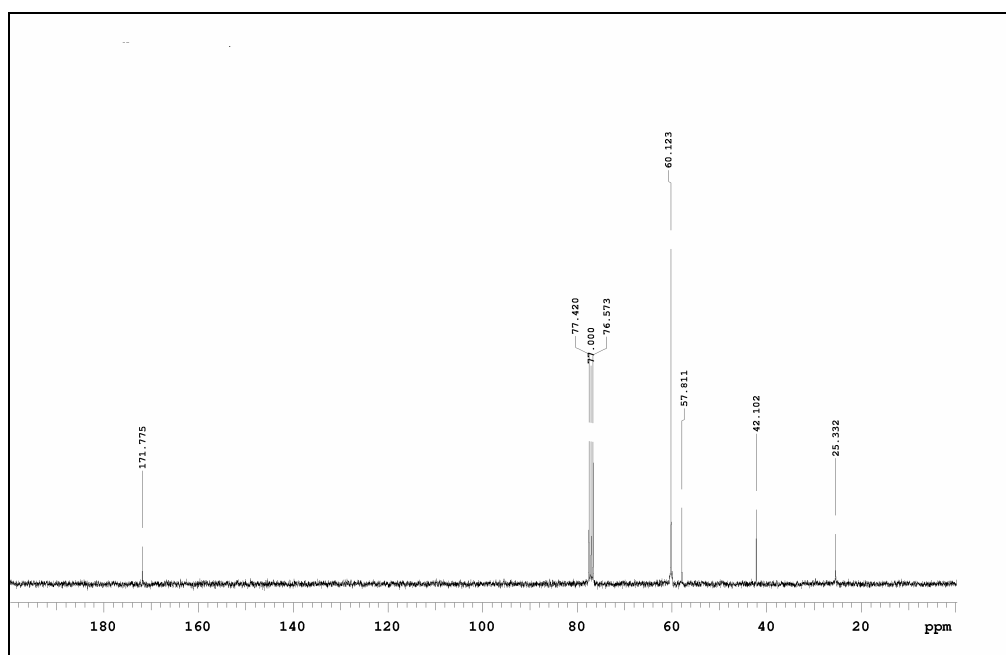
$^{13}\text{C-RMN}$ (75.4 MHz, DMSO-d_6)

 ^{13}C -DEPT

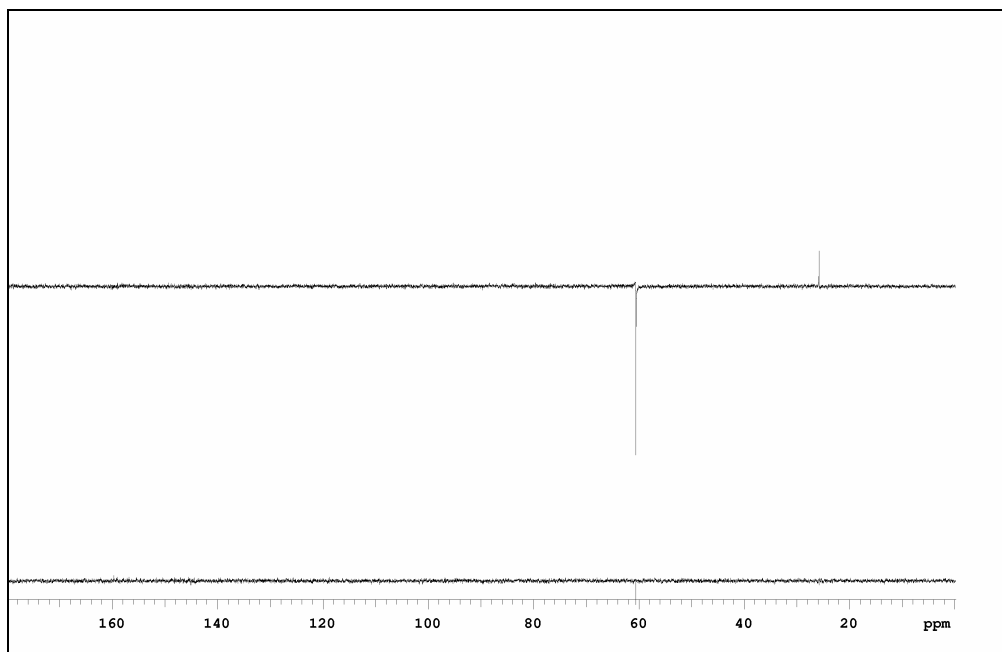
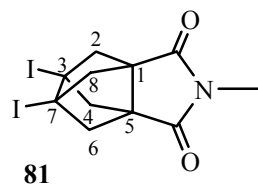
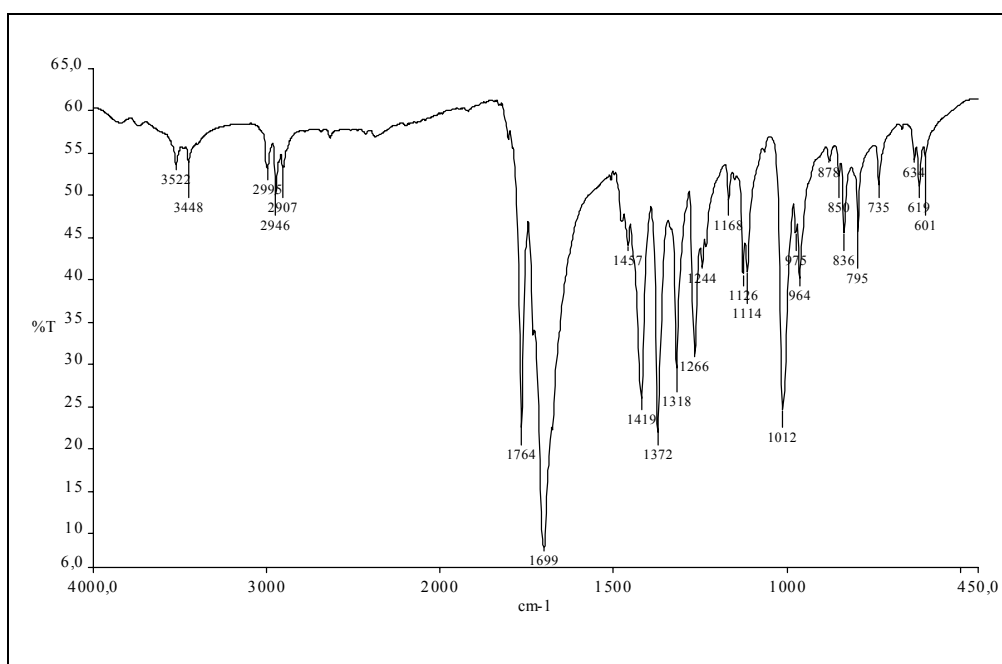
IR (KBr)



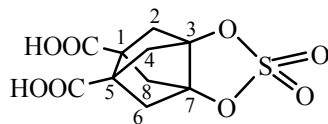
$^1\text{H-RMN}$ (300 MHz, CDCl_3)



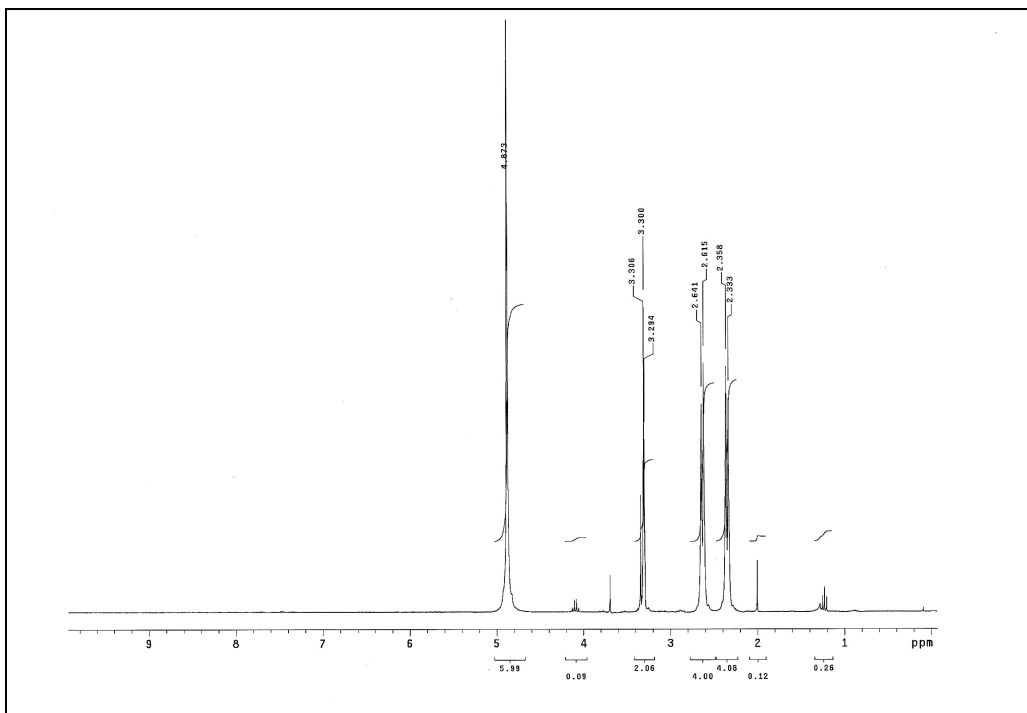
$^{13}\text{C-RMN}$ (75.4 MHz, CDCl_3)

 ^{13}C -DEPT

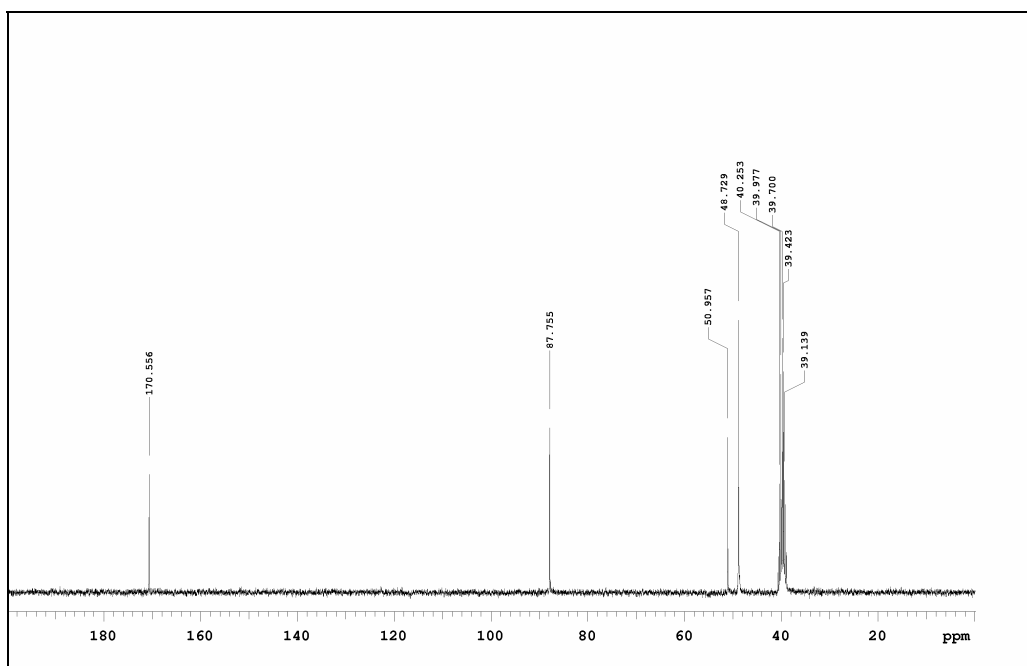
IR (KBr)



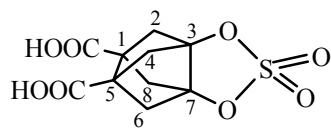
104



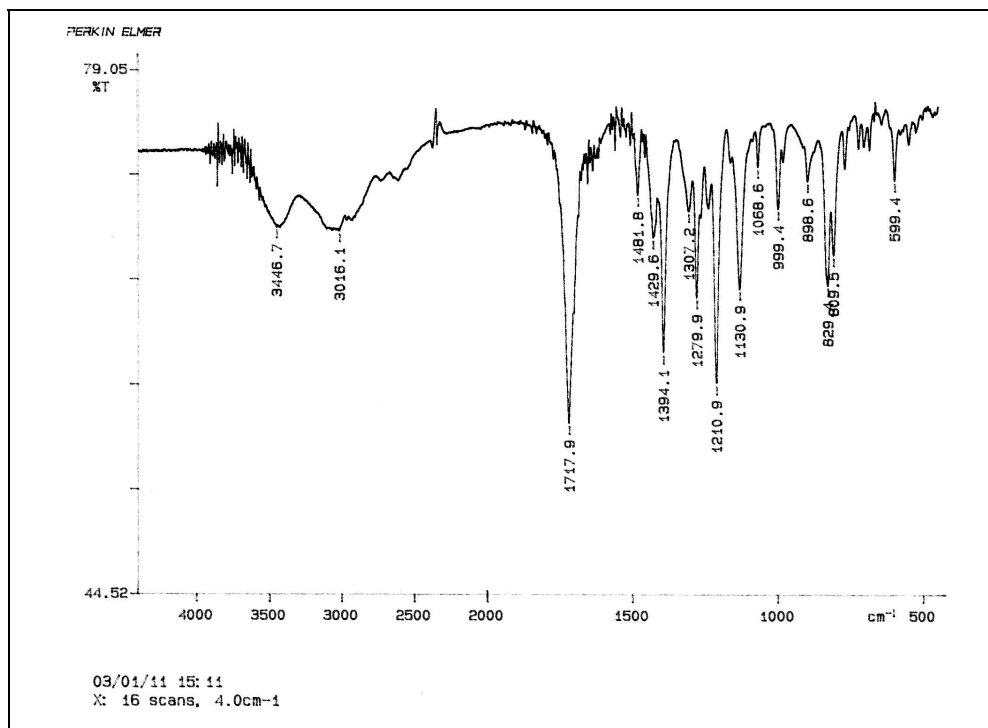
¹H-RMN (300 MHz, CD₃OD)



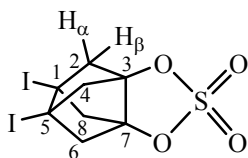
¹³C-RMN (75.4 MHz, CD₃OD)



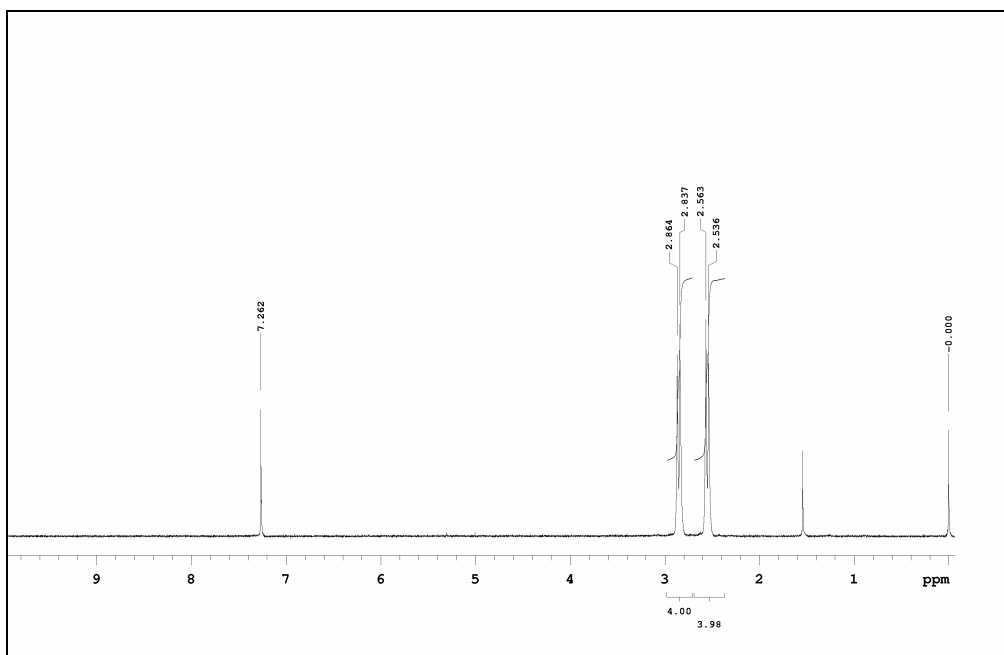
104



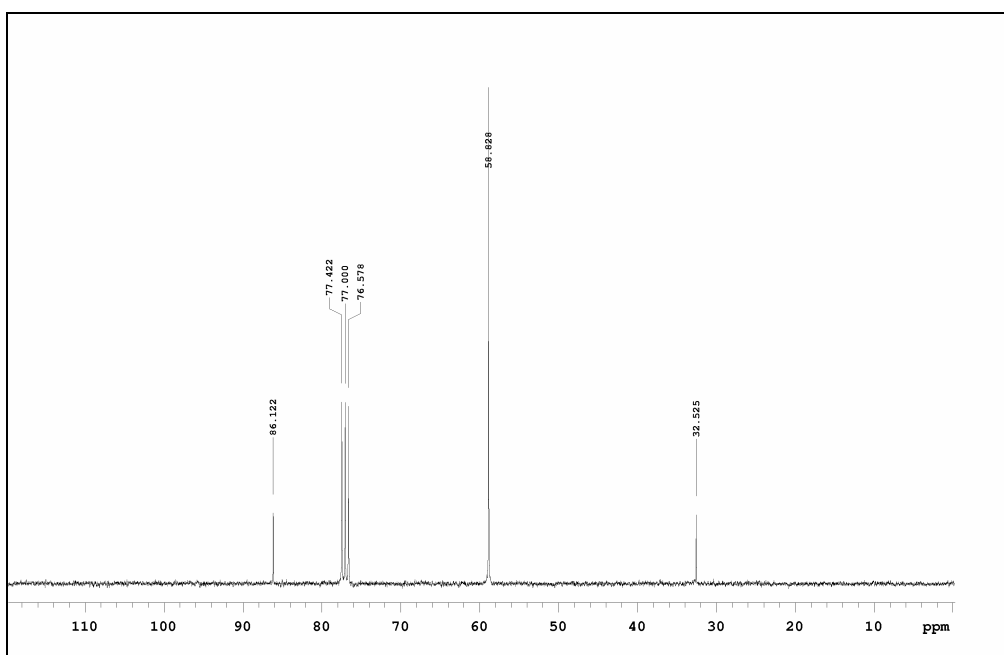
IR (KBr)



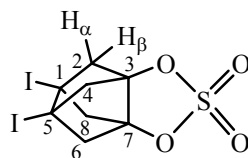
83



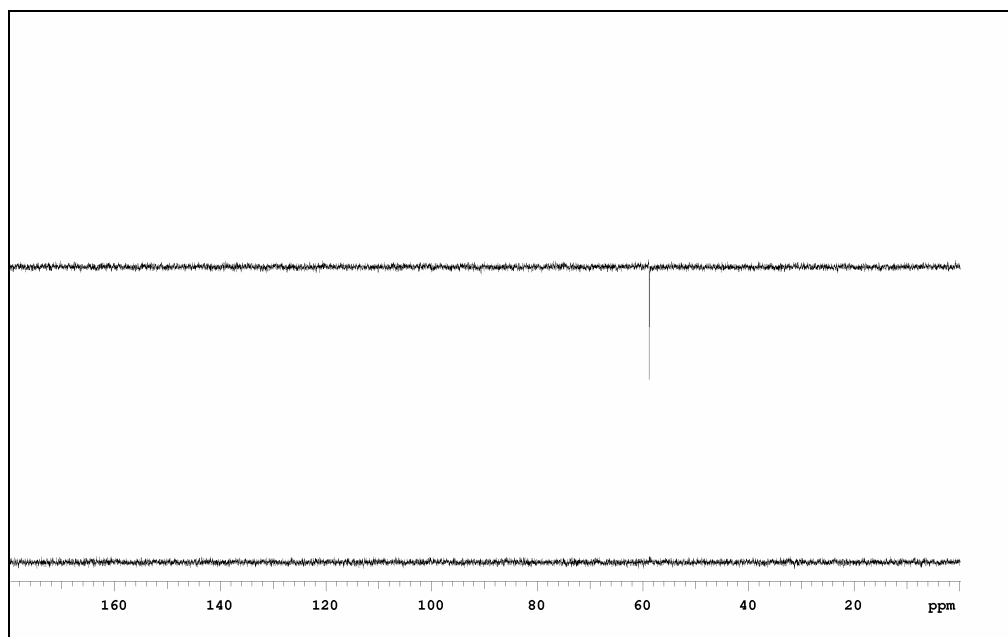
¹H-RMN (300 MHz, CDCl₃)



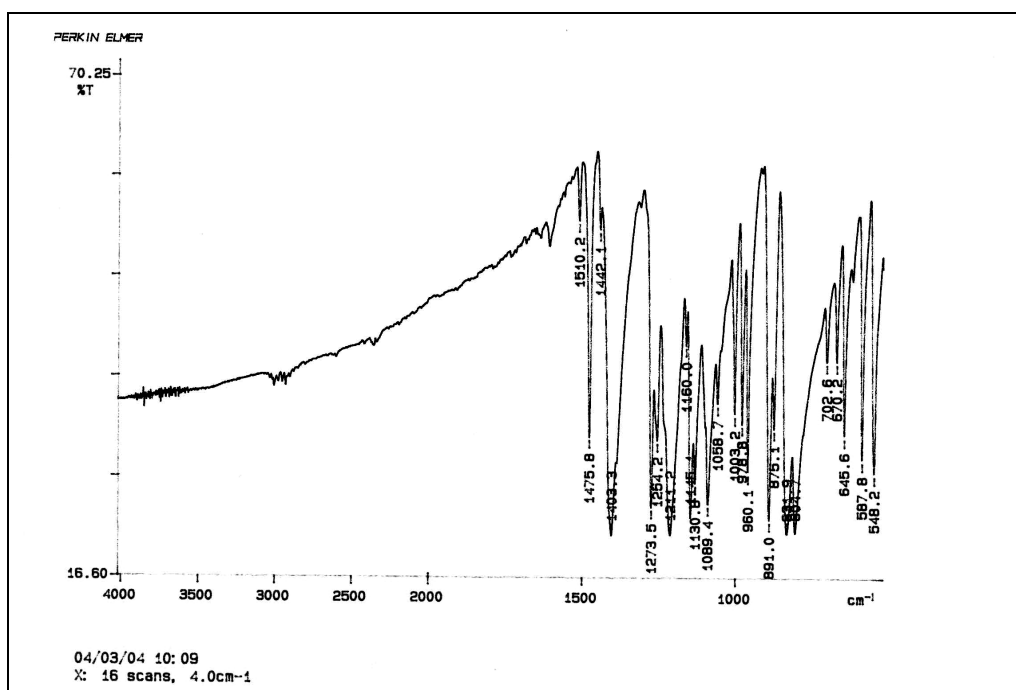
¹³C-RMN (75.4 MHz, CDCl₃)



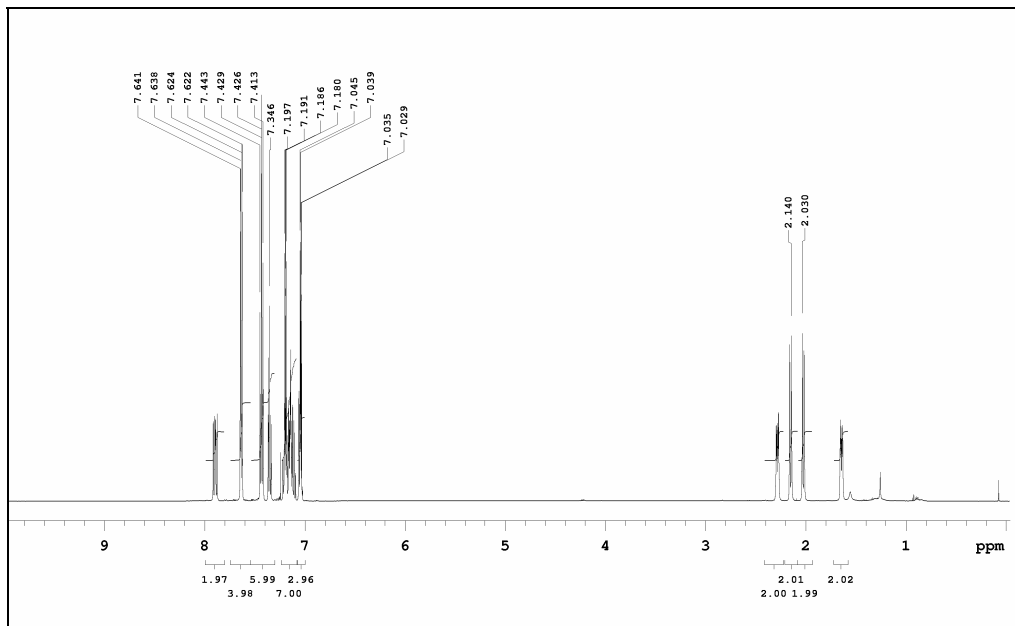
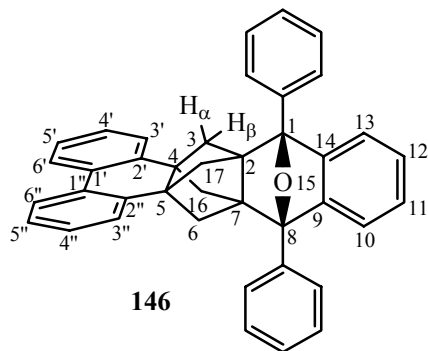
83



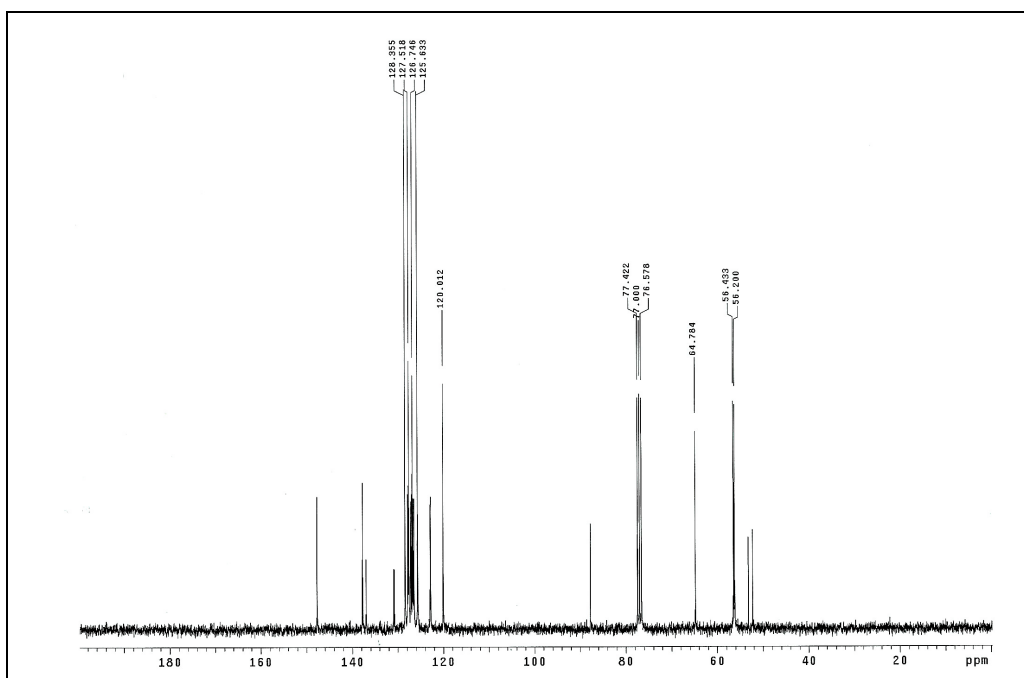
^{13}C -DEPT (75.4 MHz, CDCl_3)



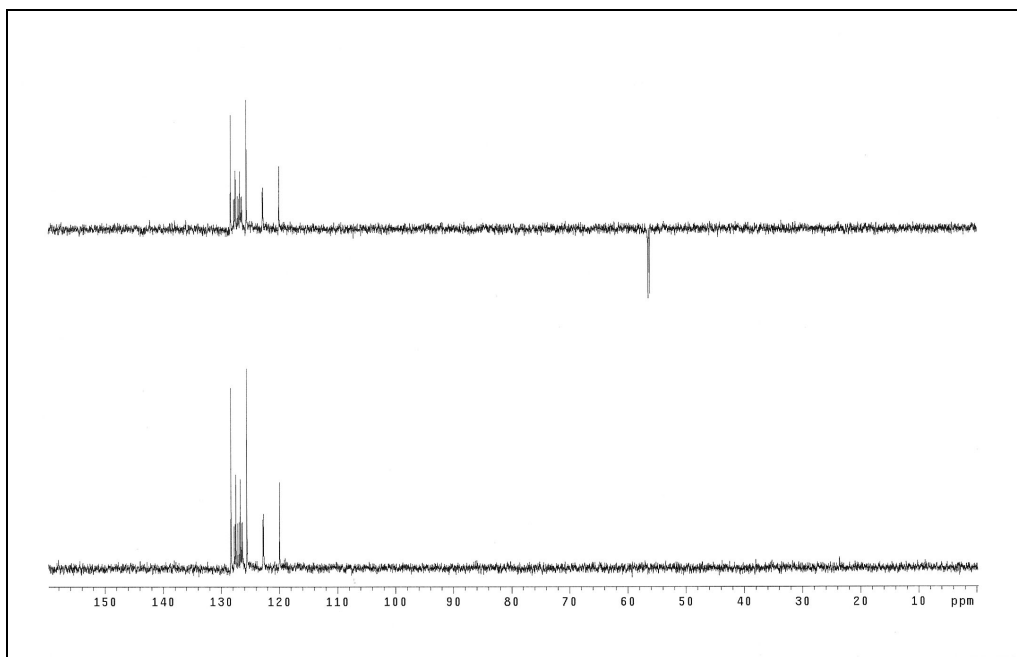
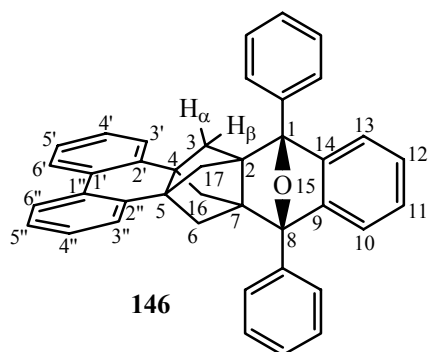
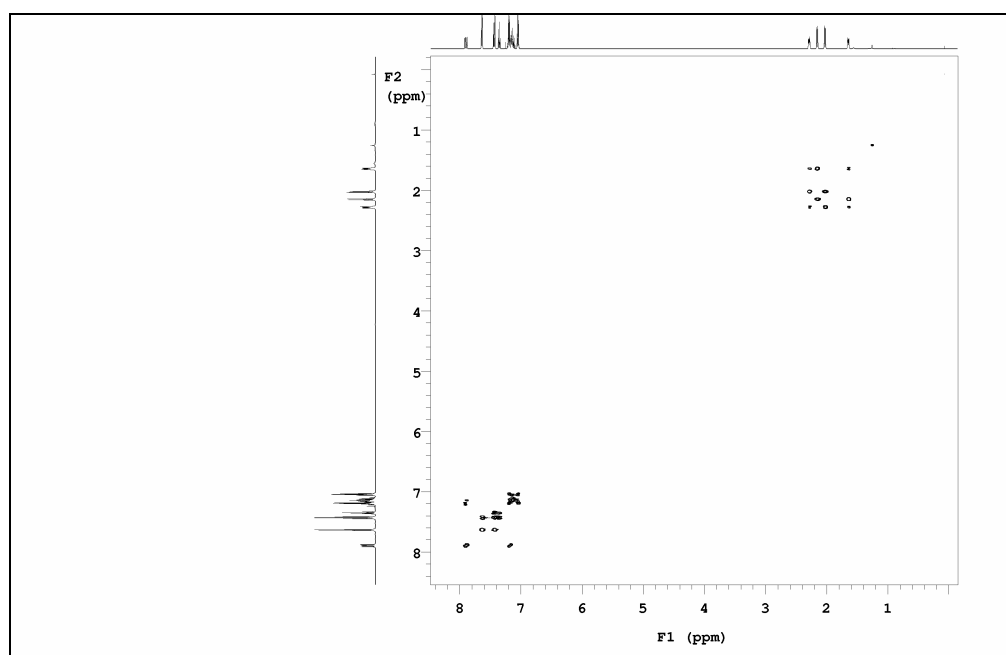
IR (KBr)

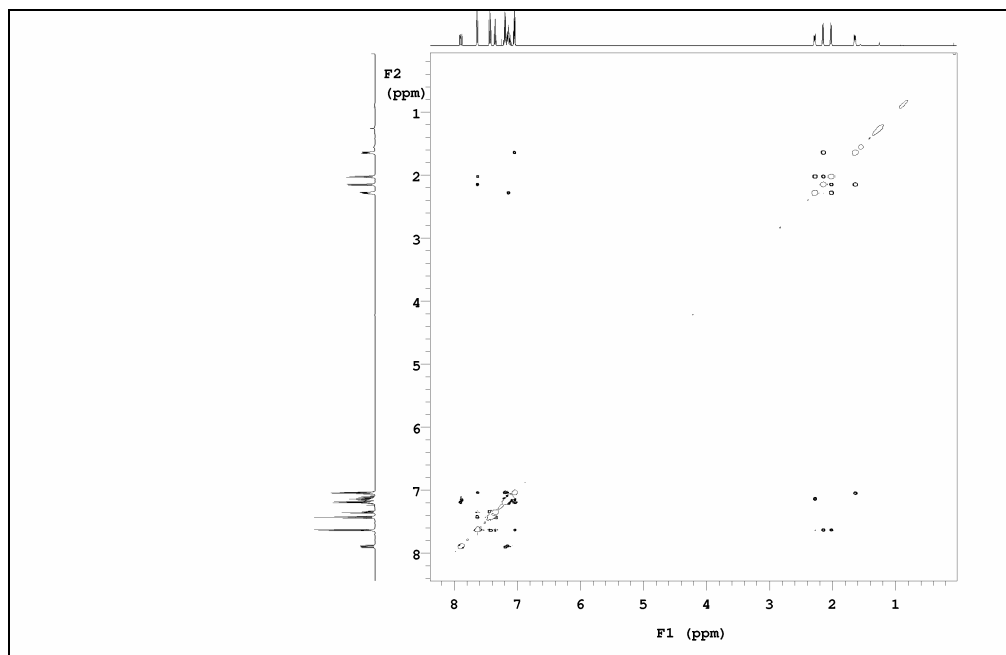
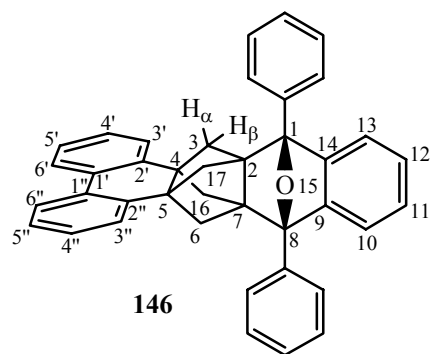


¹H-RMN (500 MHz, CDCl₃)

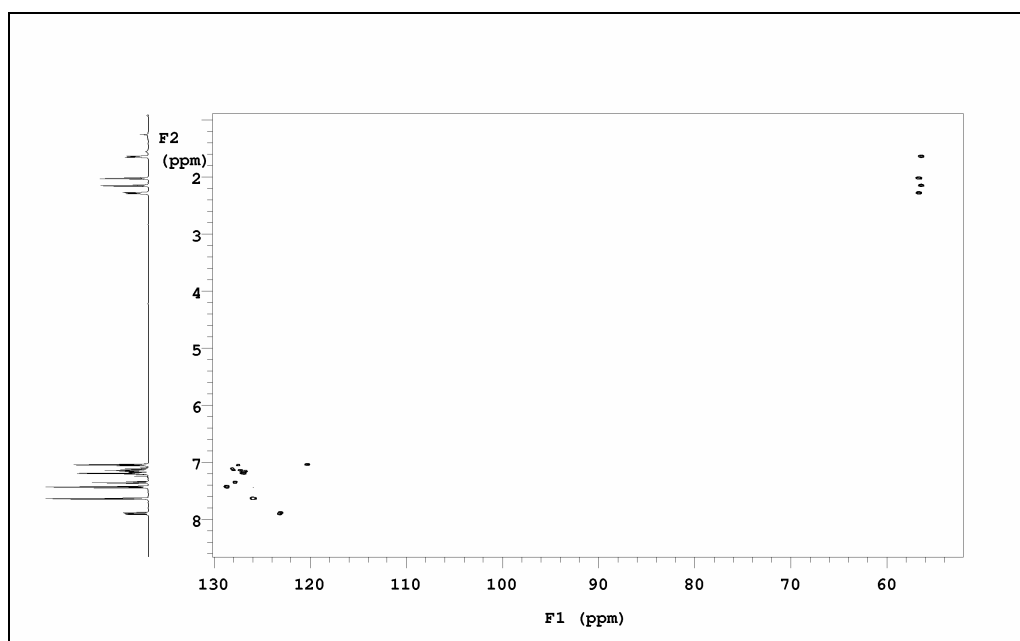


¹³C-RMN (75.4 MHz, CDCl₃)

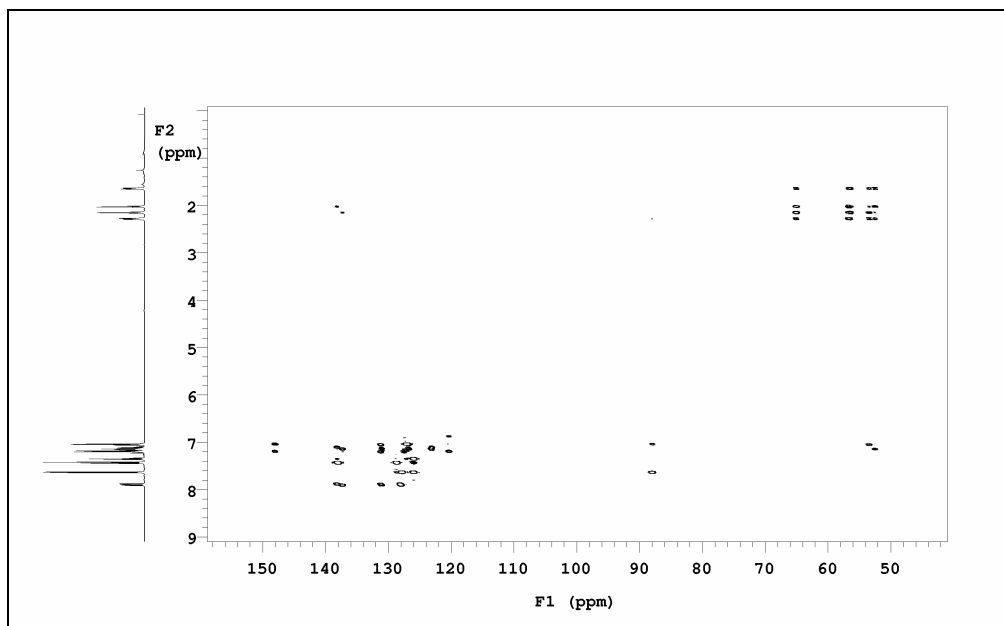
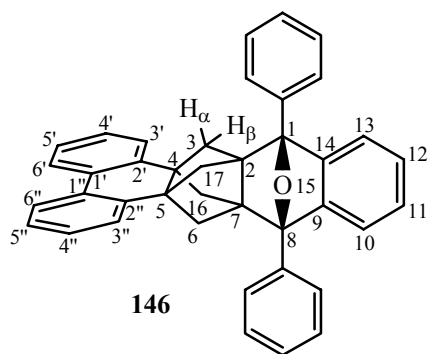
 ^{13}C -DEPT ^1H - ^1H -COSY



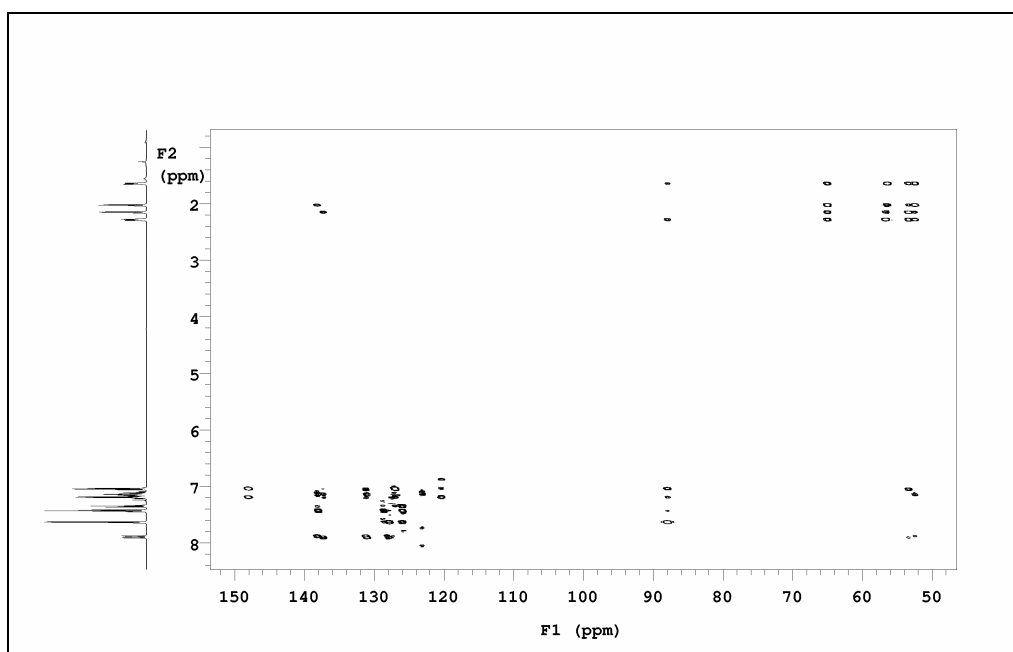
$^1\text{H}-^1\text{H}$ -NOESY



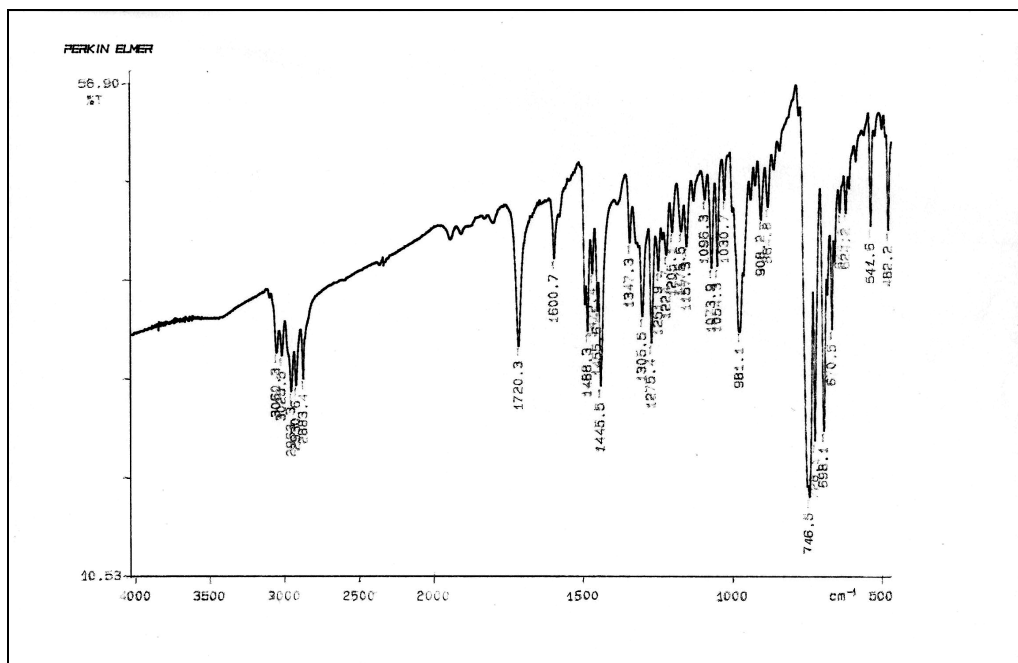
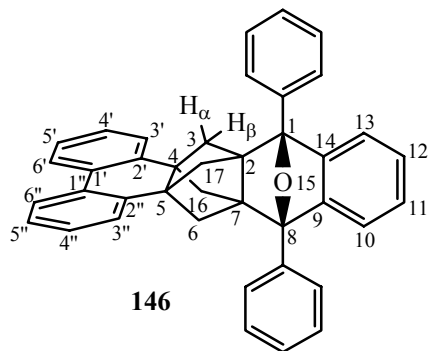
$^1\text{H}-^{13}\text{C}$ -HSQC



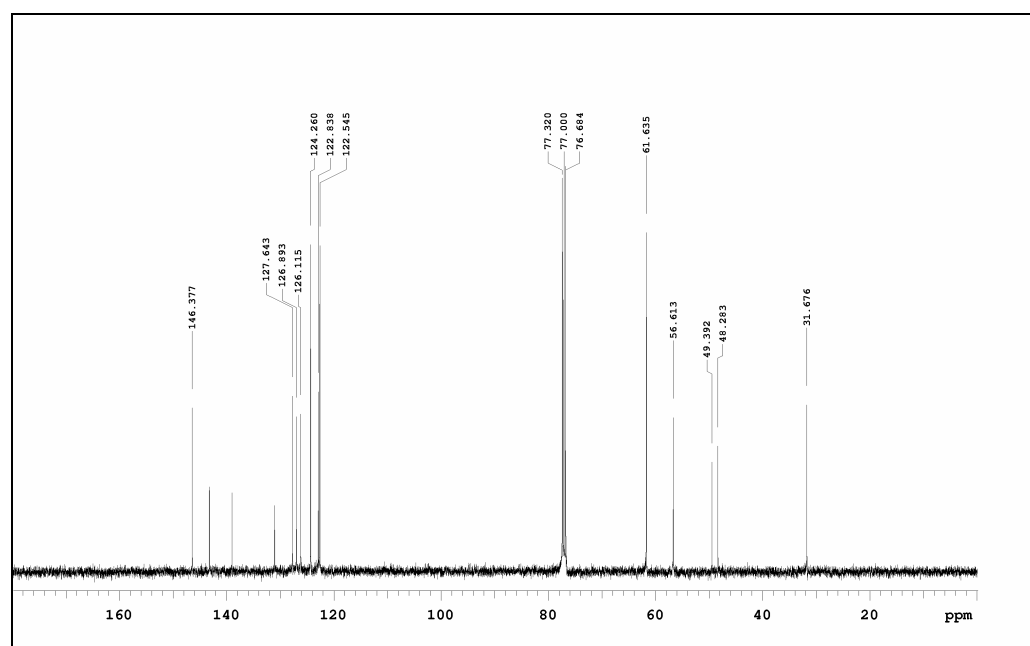
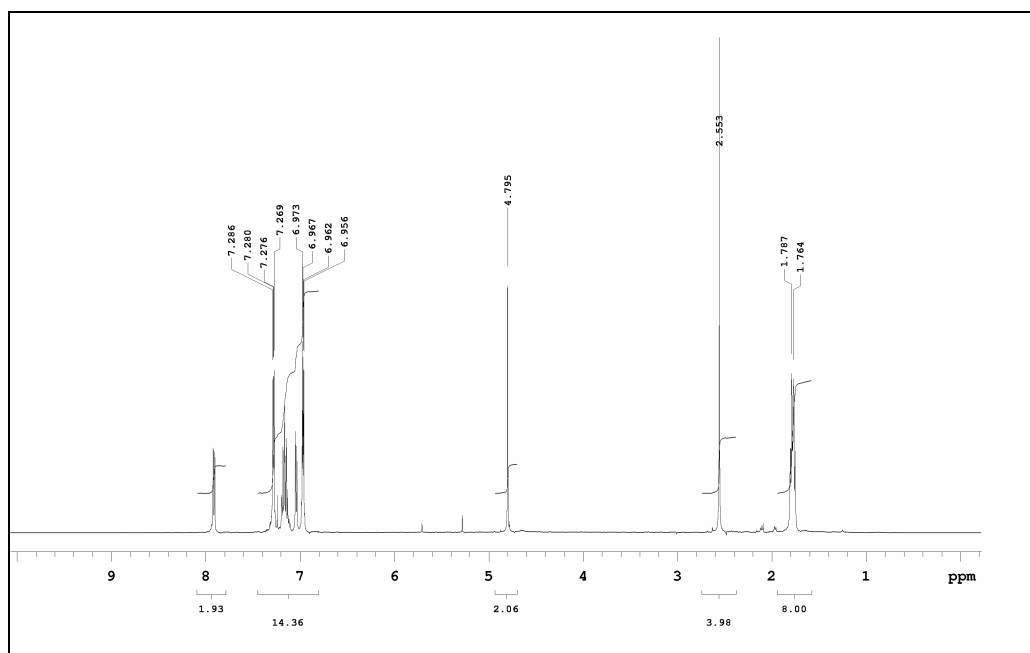
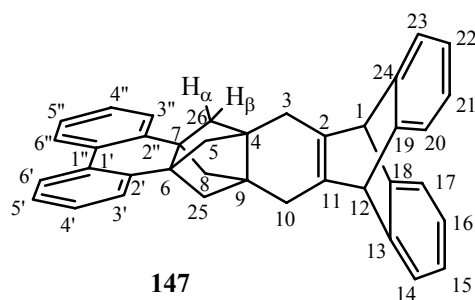
$^1\text{H}-^{13}\text{C}\text{-HMBC } J = 8 \text{ Hz}$

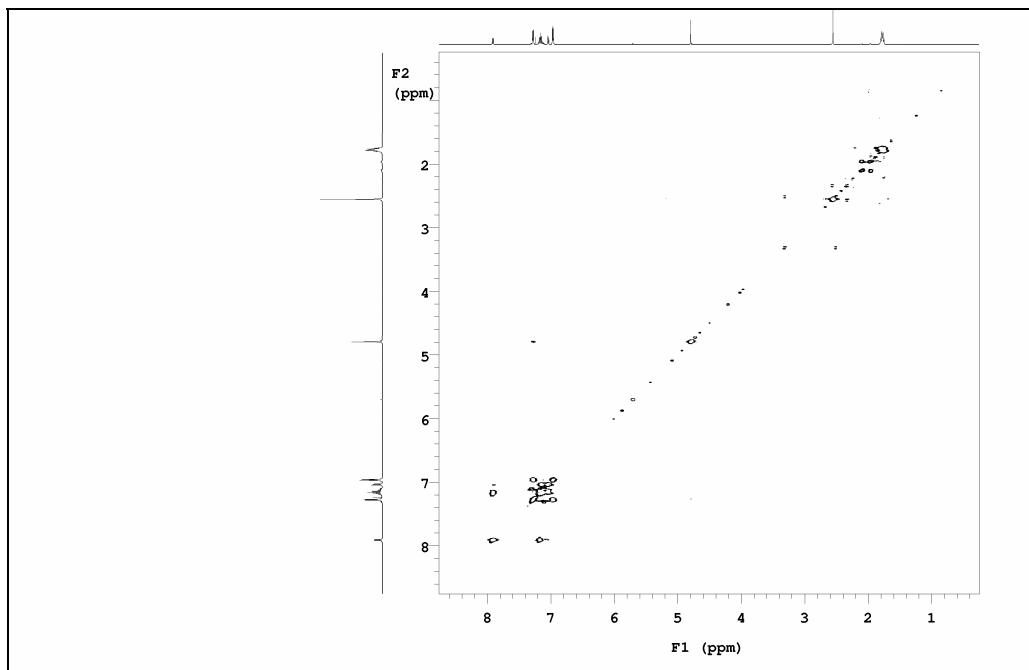
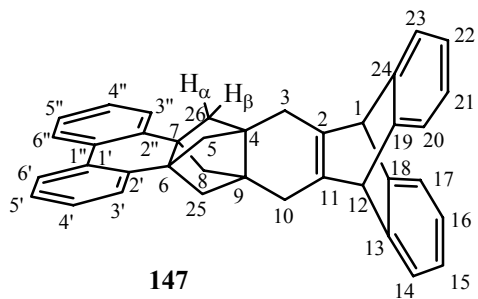


$^1\text{H}-^{13}\text{C}\text{-HMBC } J = 5 \text{ Hz}$

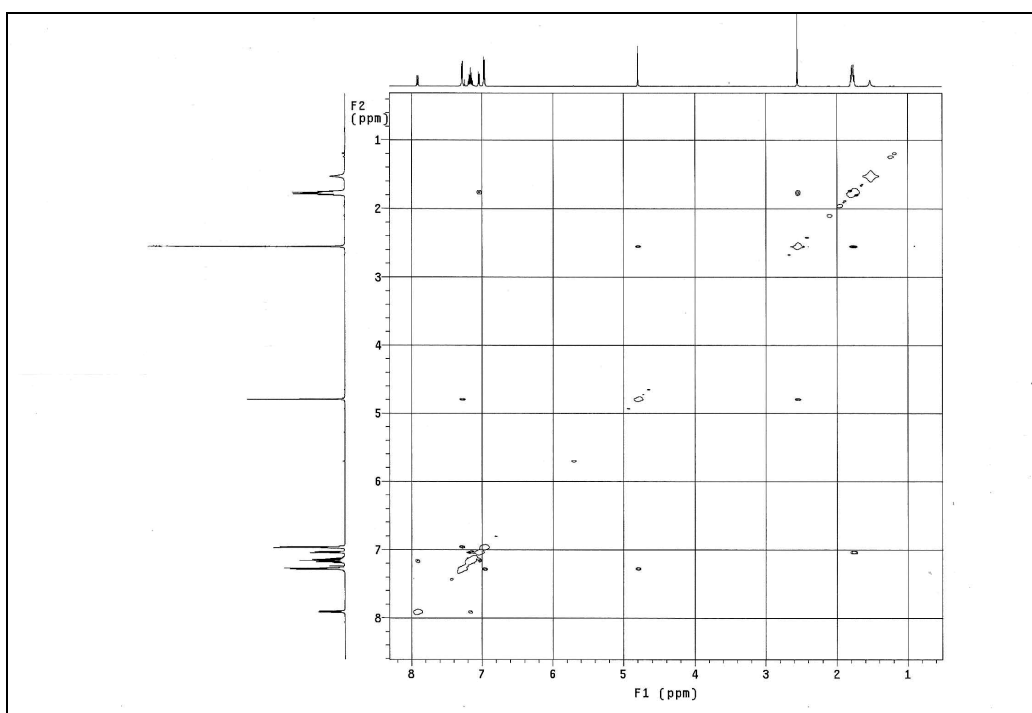


IR (KBr)

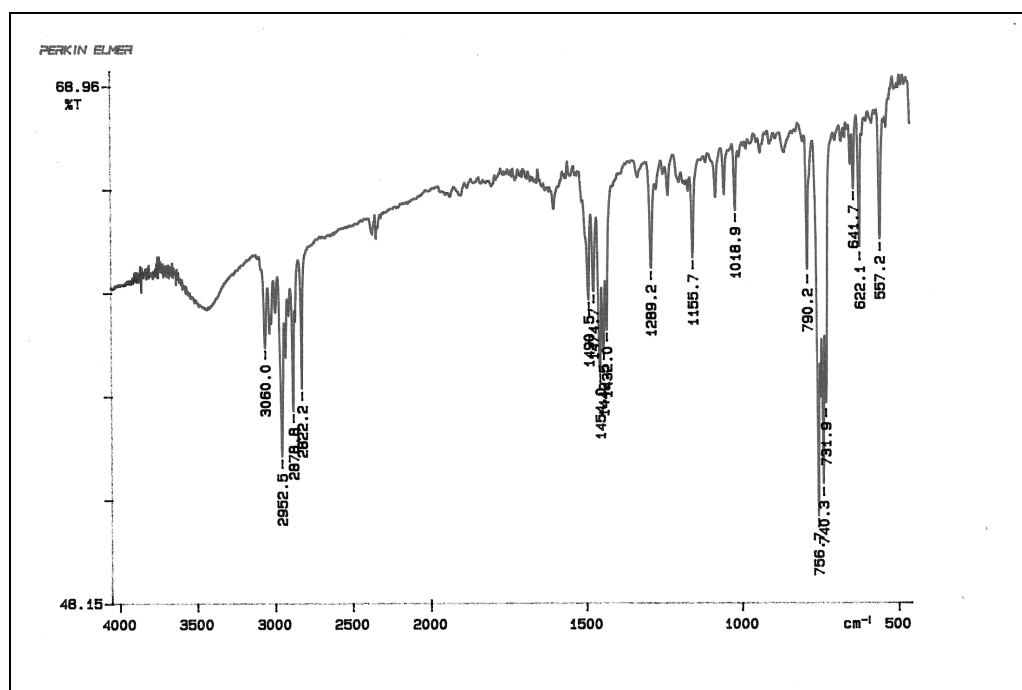
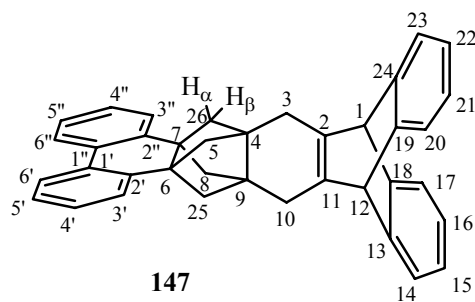




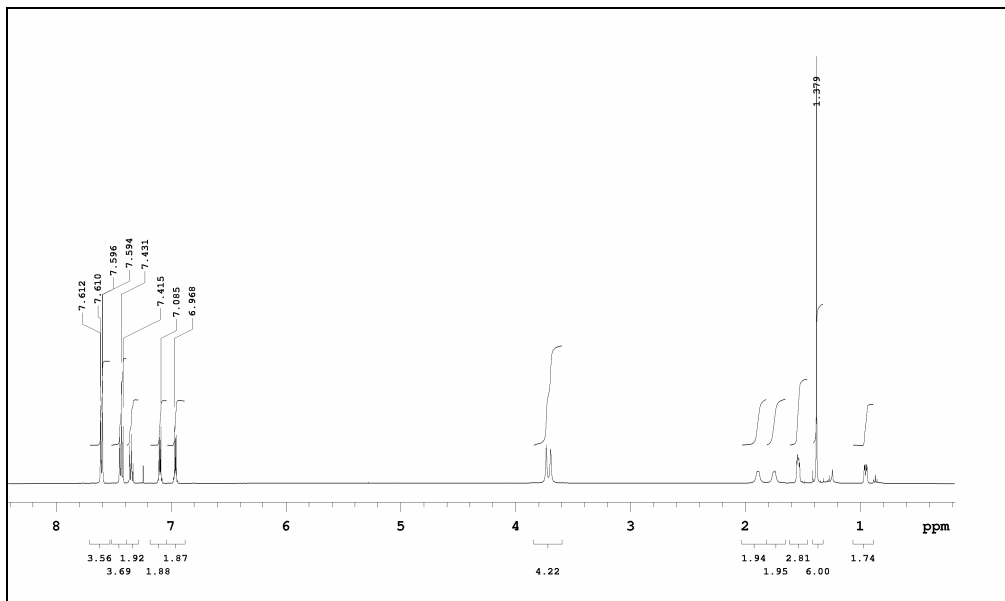
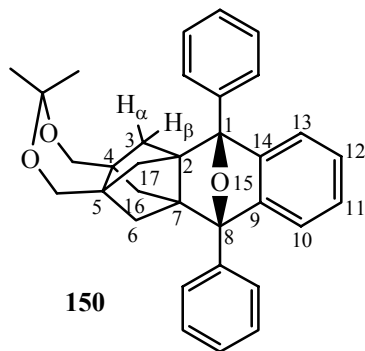
$^1\text{H}-^1\text{H-COSY}$



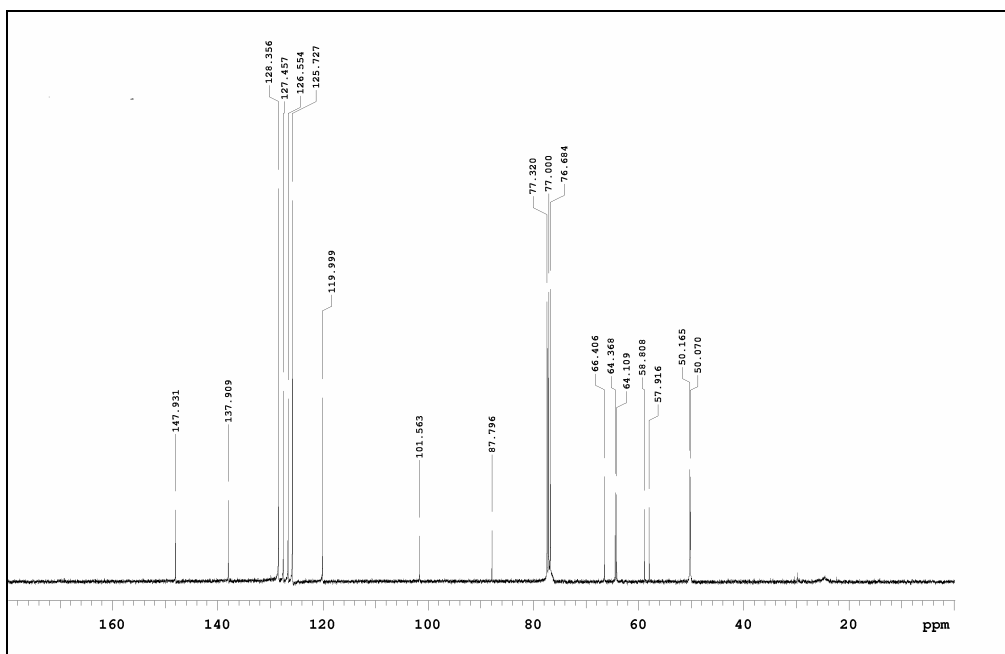
$^1\text{H}-^1\text{H-NOESY}$



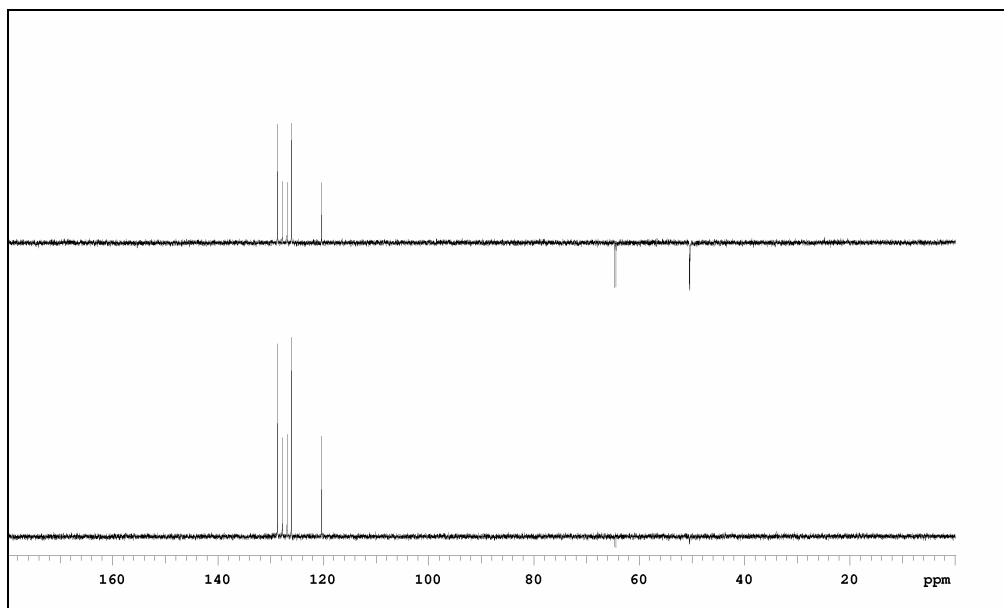
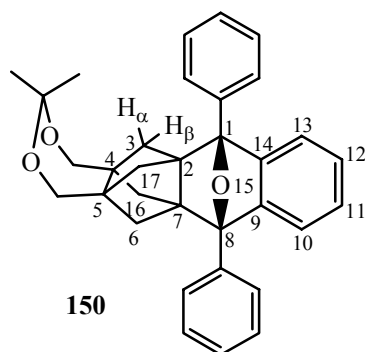
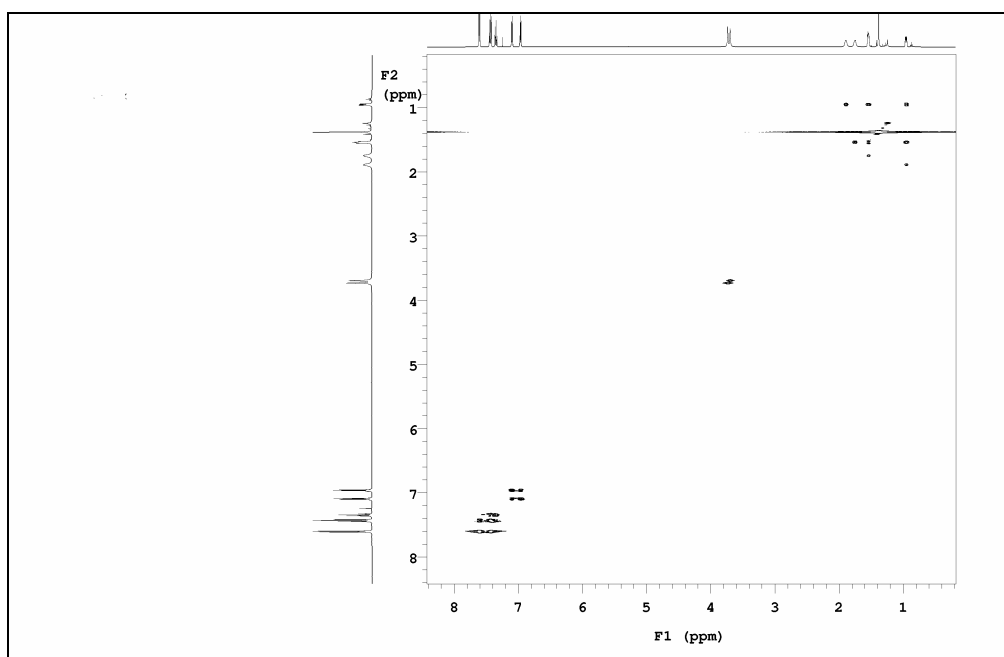
IR (KBr)

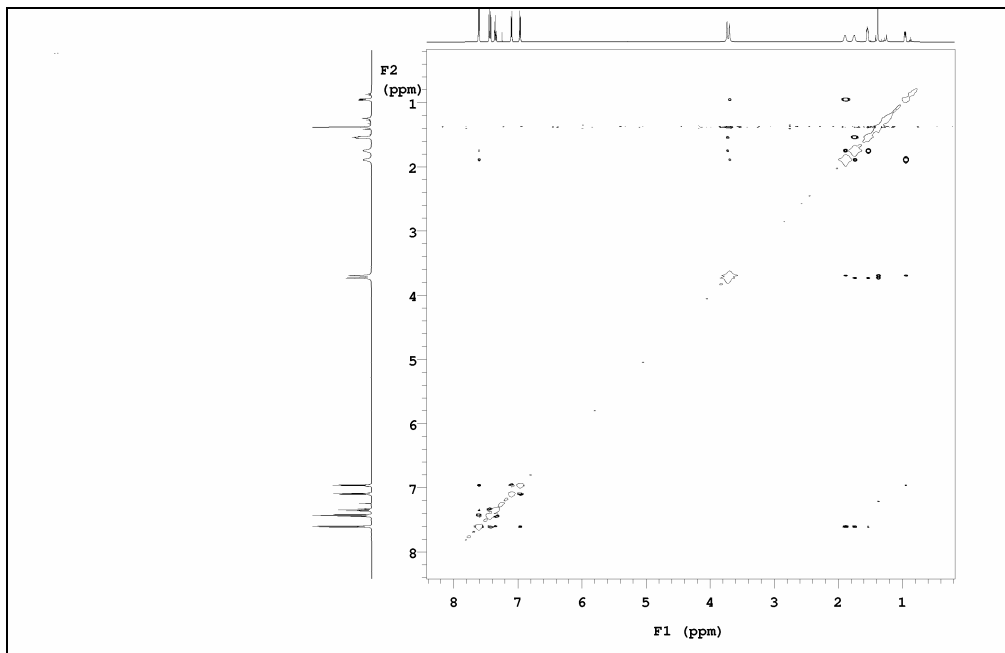
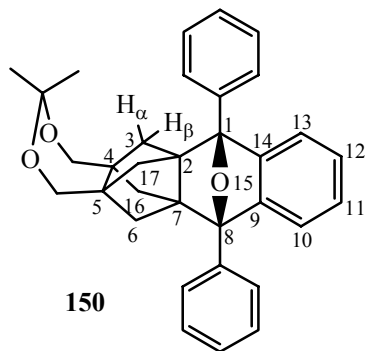


¹H-RMN (500 MHz, CDCl₃)

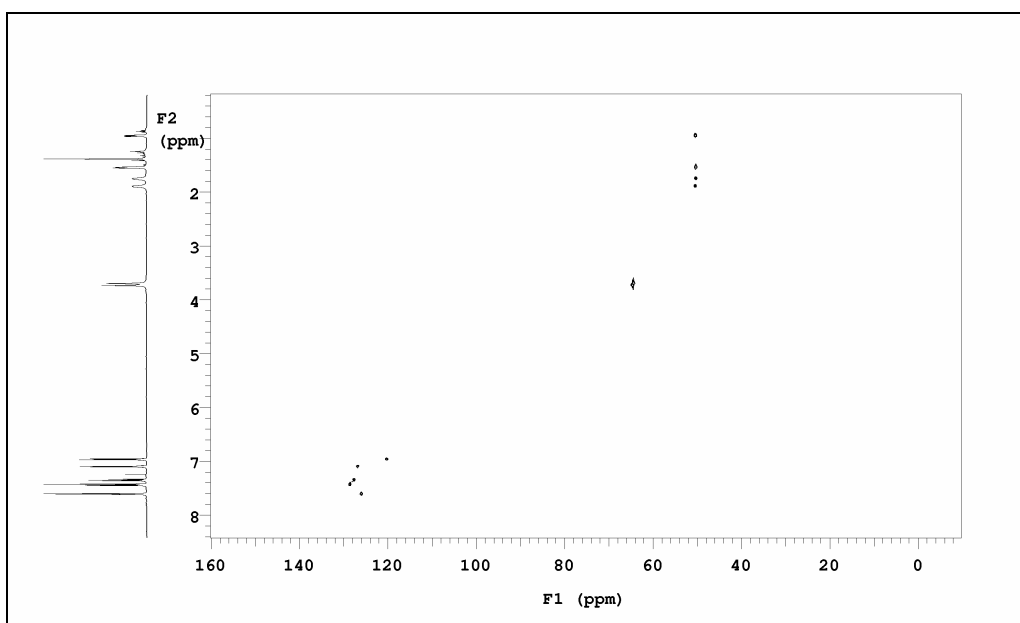


¹³C-RMN (100.6 MHz, CDCl₃)

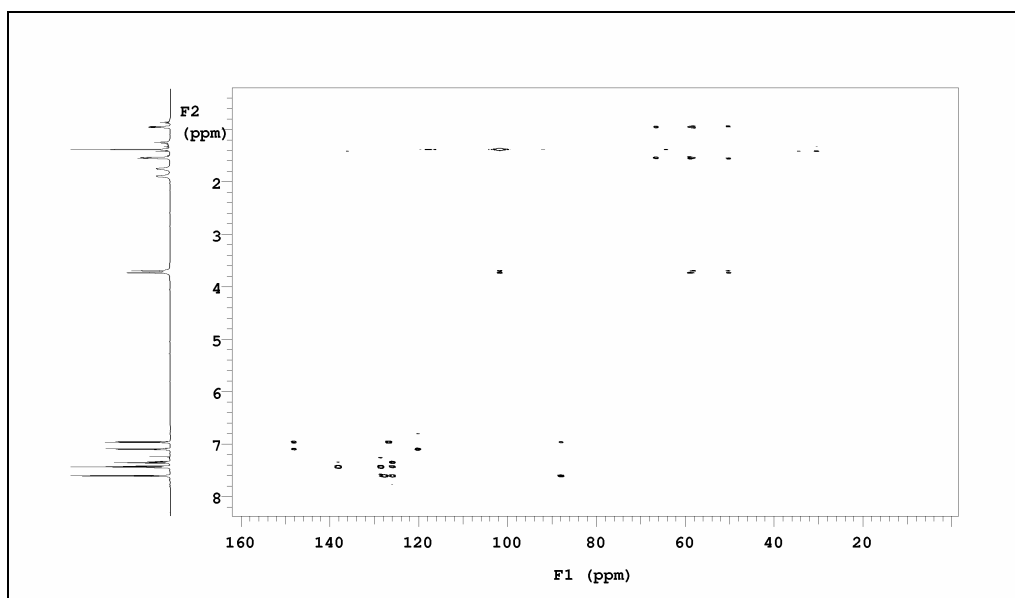
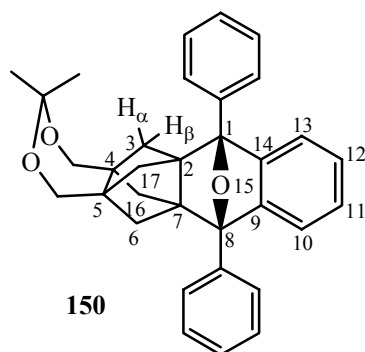
 ^{13}C -DEPT ^1H - ^1H -COSY



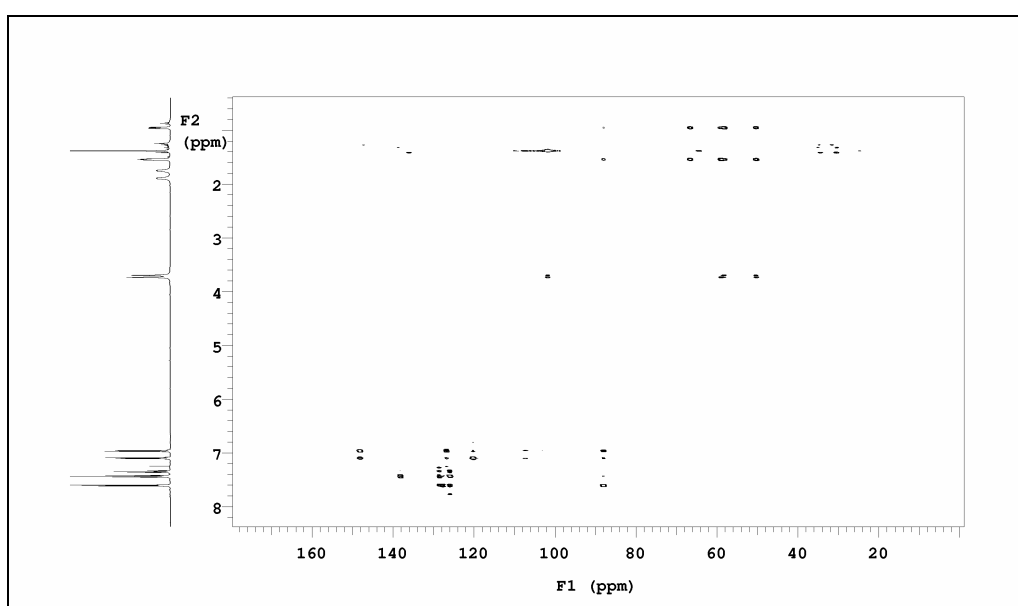
$^1\text{H}-^1\text{H}$ -NOESY



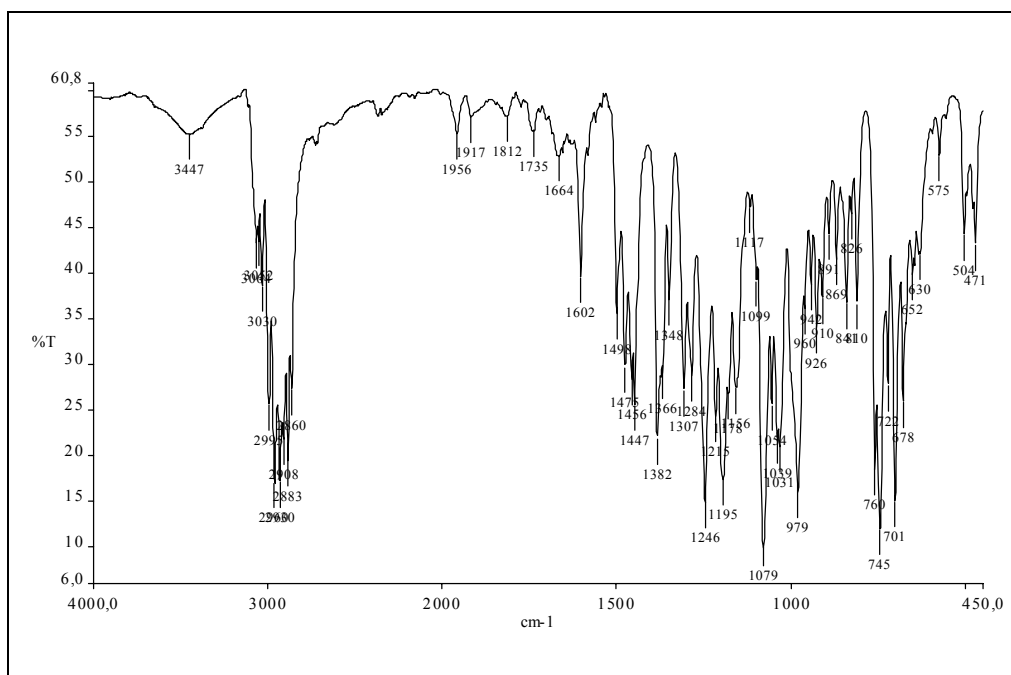
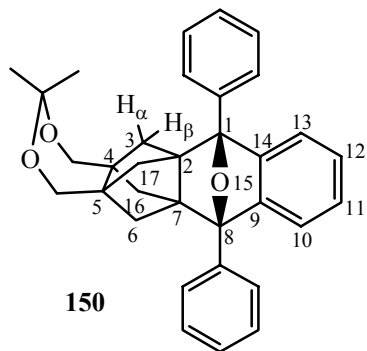
$^1\text{H}-^{13}\text{C}$ -HSQC

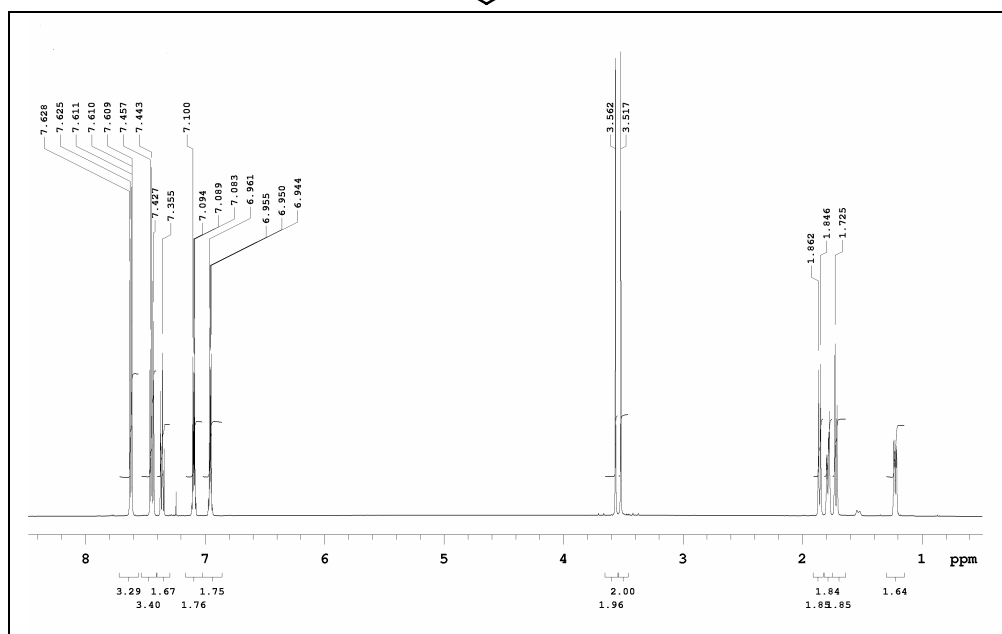
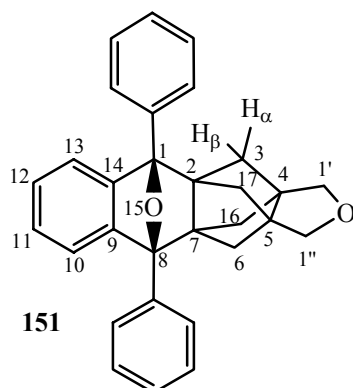
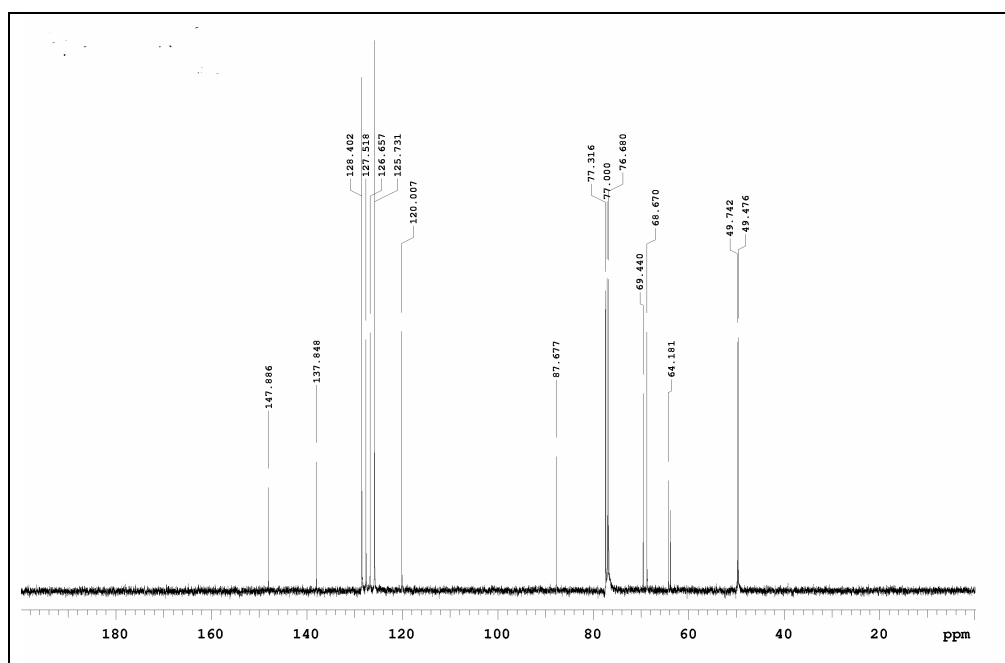


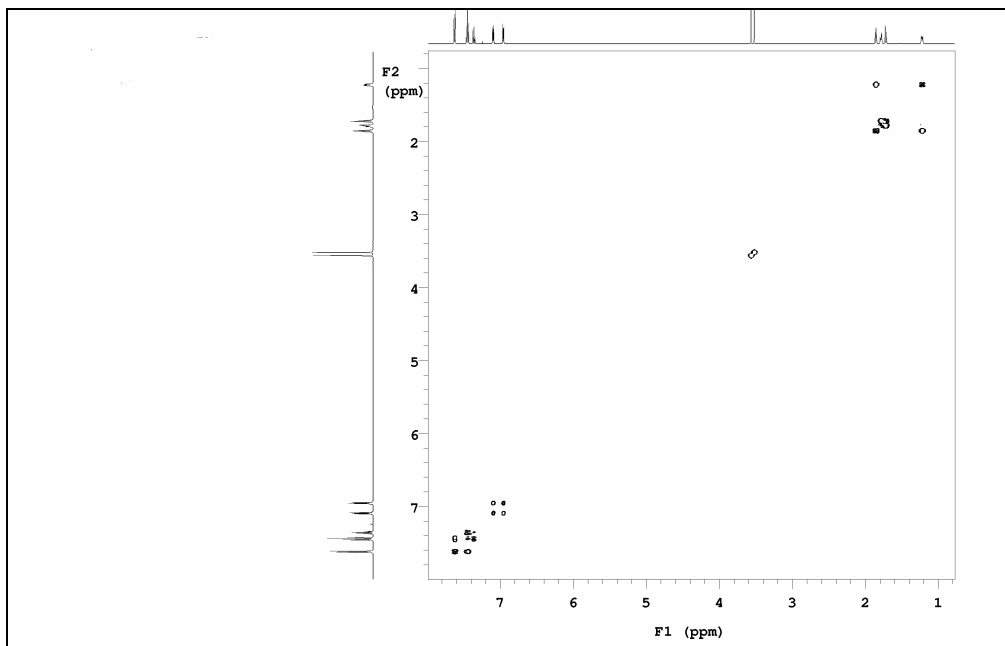
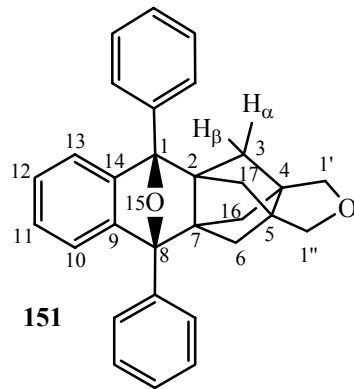
$^1\text{H}-^{13}\text{C}\text{-HMBC } J = 8 \text{ Hz}$



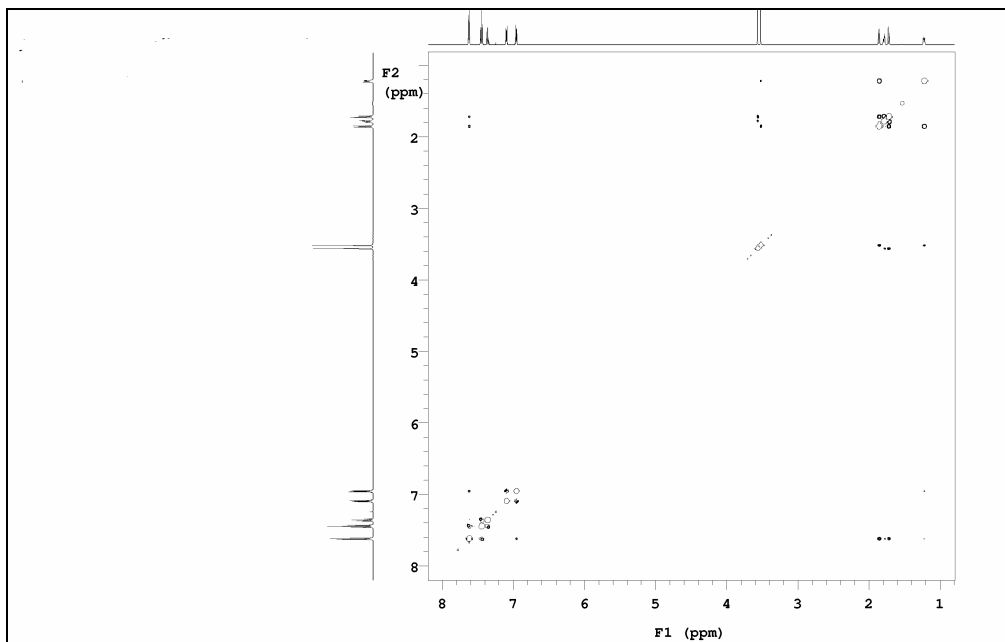
$^1\text{H}-^{13}\text{C}\text{-HMBC } J = 5 \text{ Hz}$



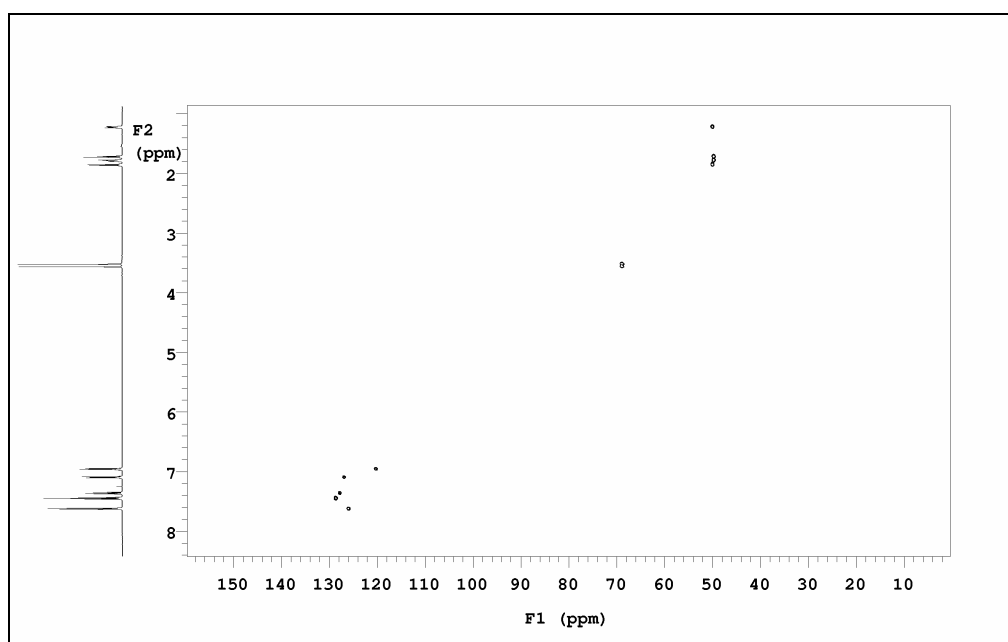
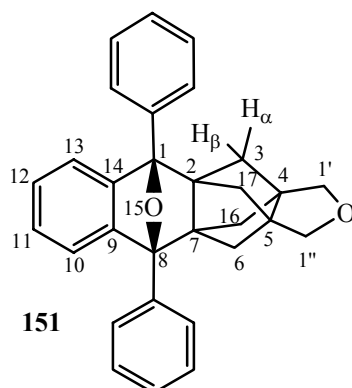
 $^1\text{H-RMN}$ (500 MHz, CDCl_3) $^{13}\text{C-RMN}$ (100.6 MHz, CDCl_3)



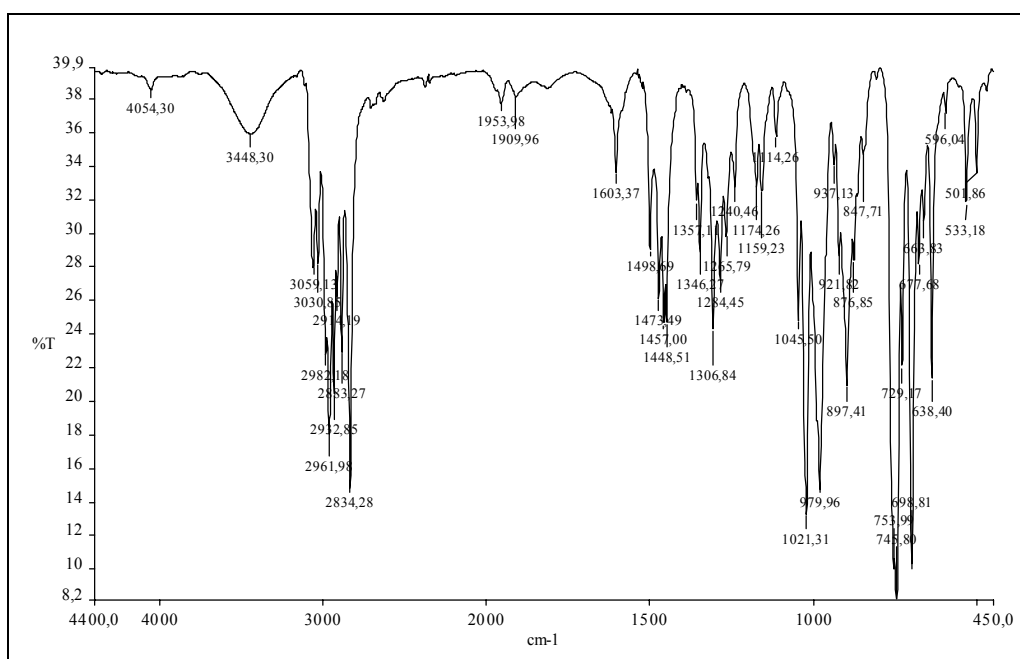
$^1\text{H}-^1\text{H-COSY}$



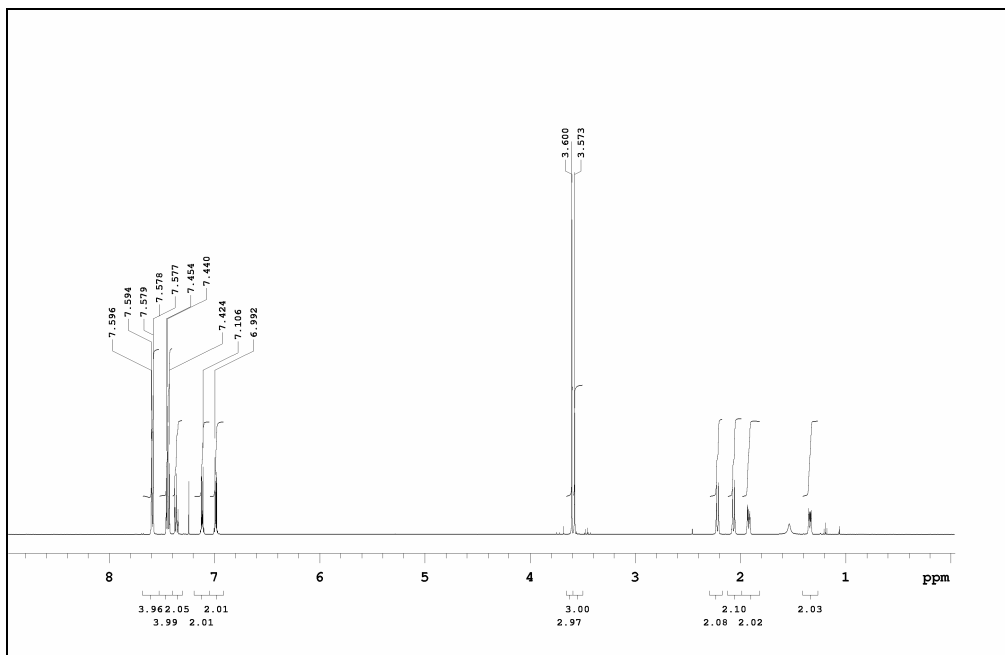
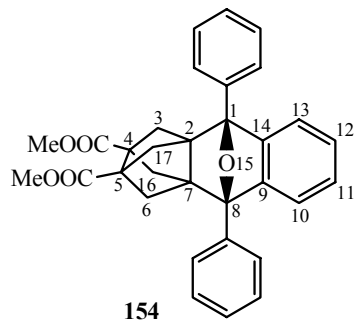
$^1\text{H}-^1\text{H-NOESY}$



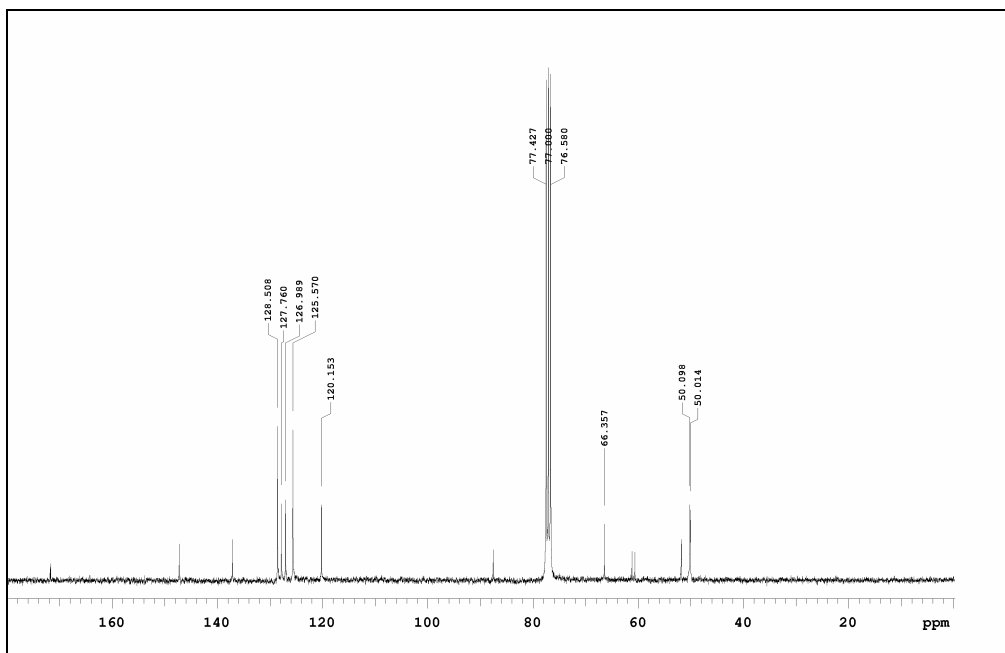
$^1\text{H}-^{13}\text{C}$ -HSQC



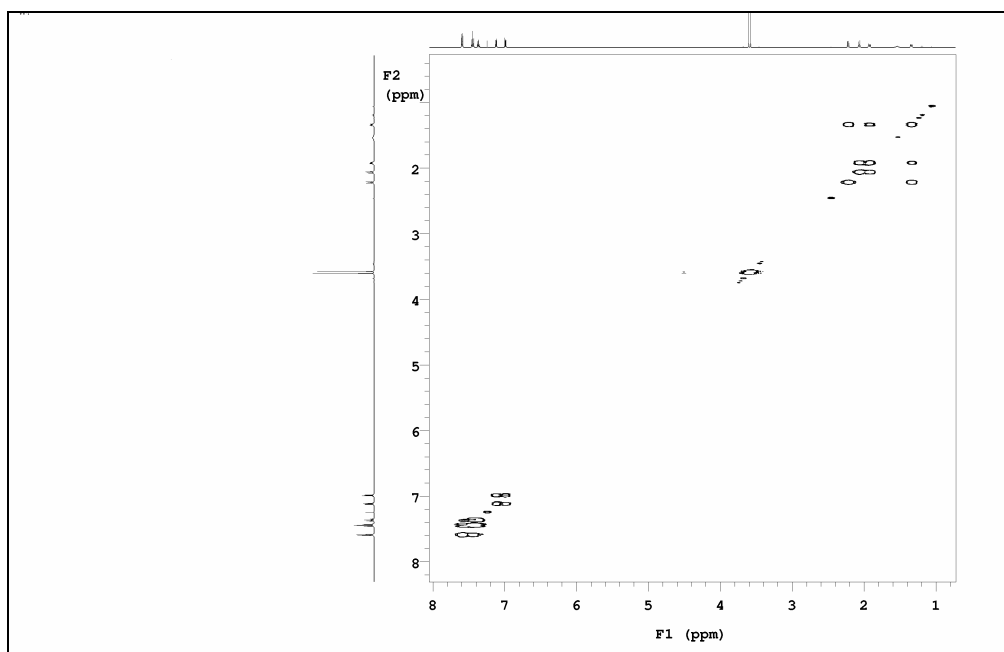
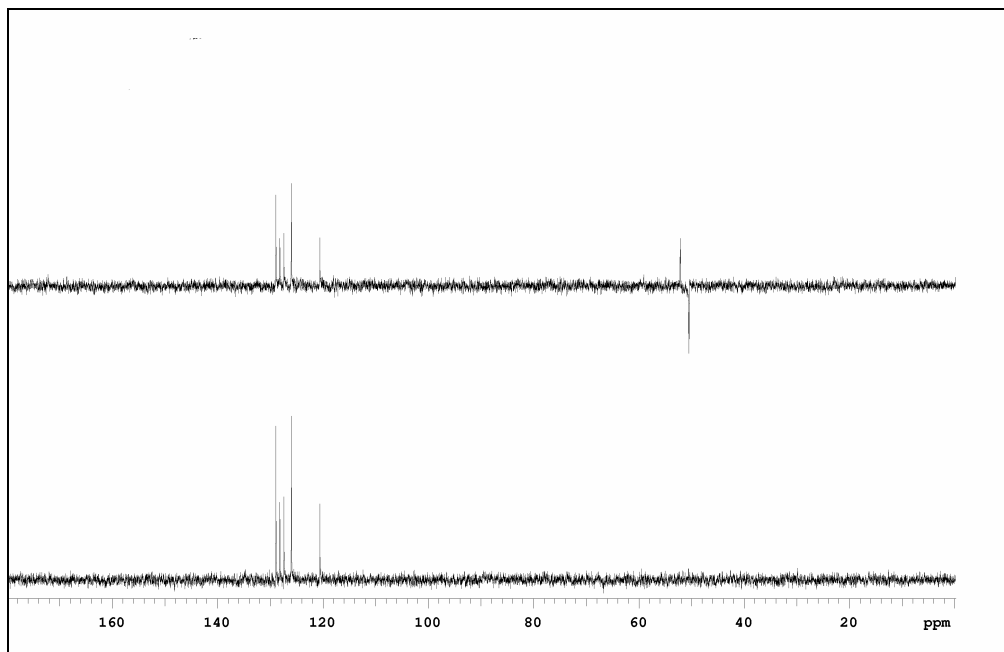
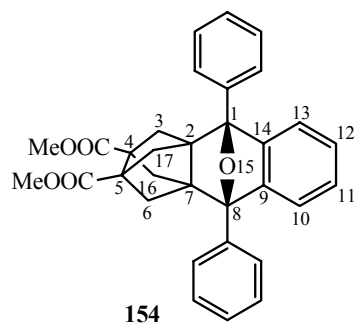
IR (KBr)

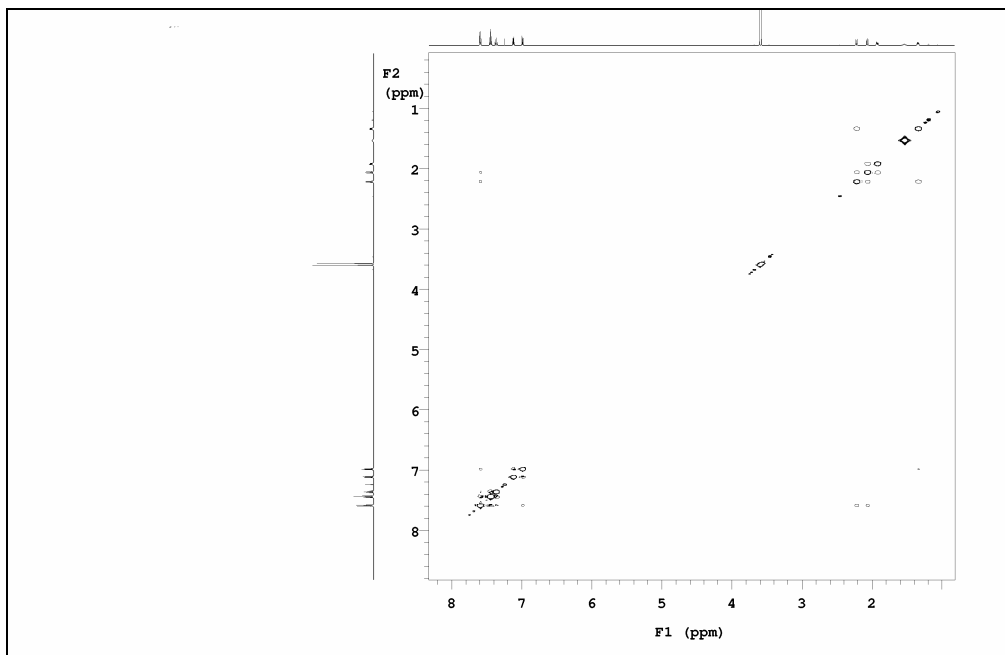
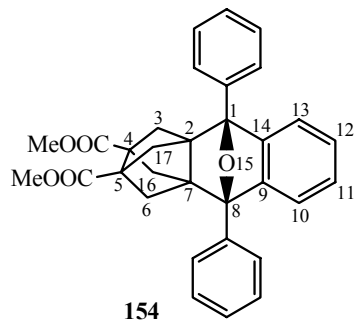


¹H-RMN (500 MHz, CDCl₃)

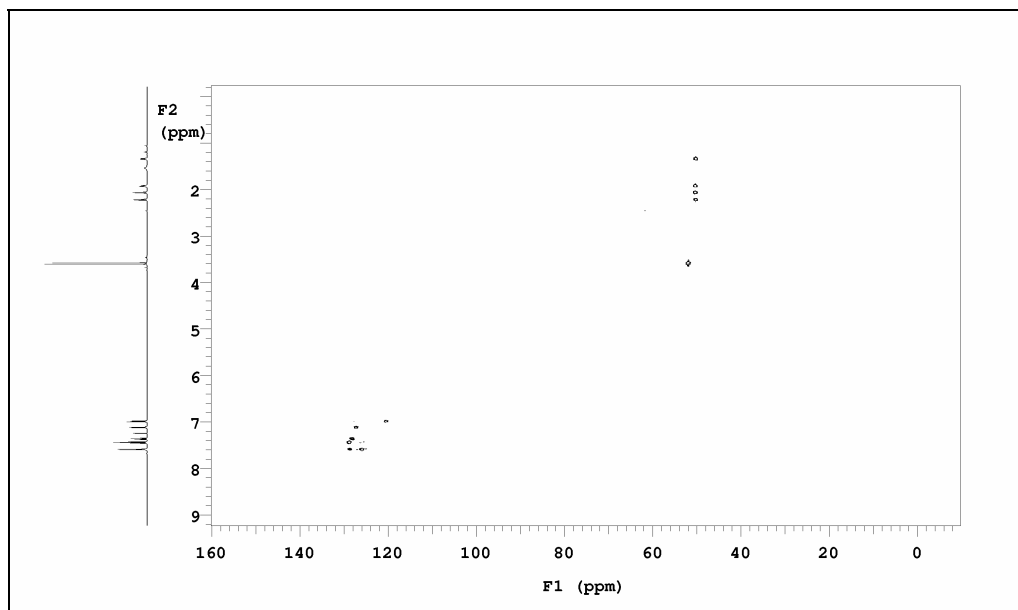


¹³C-RMN (75.4 MHz, CDCl₃)

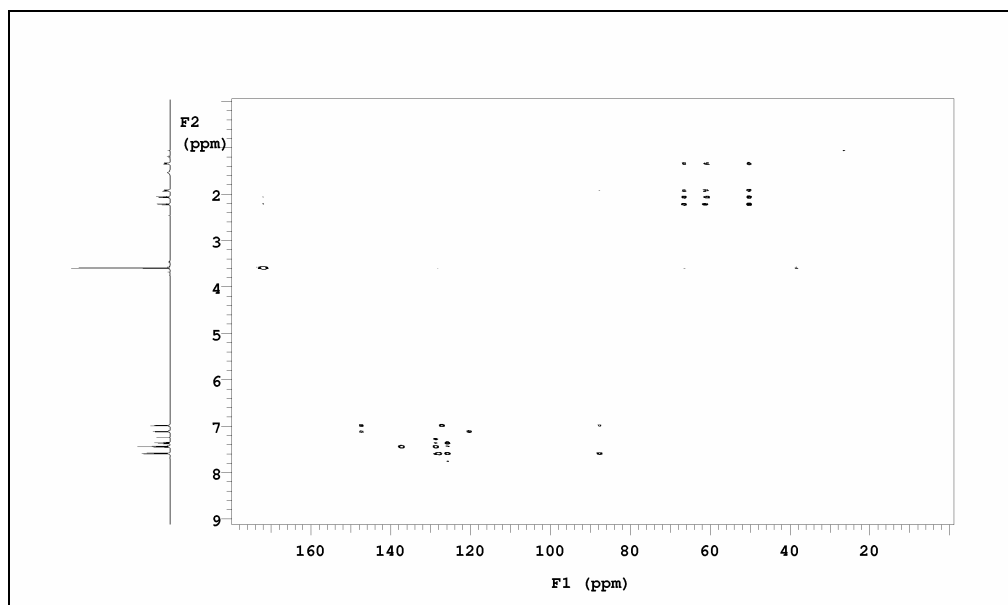
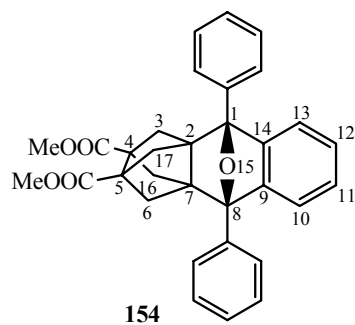
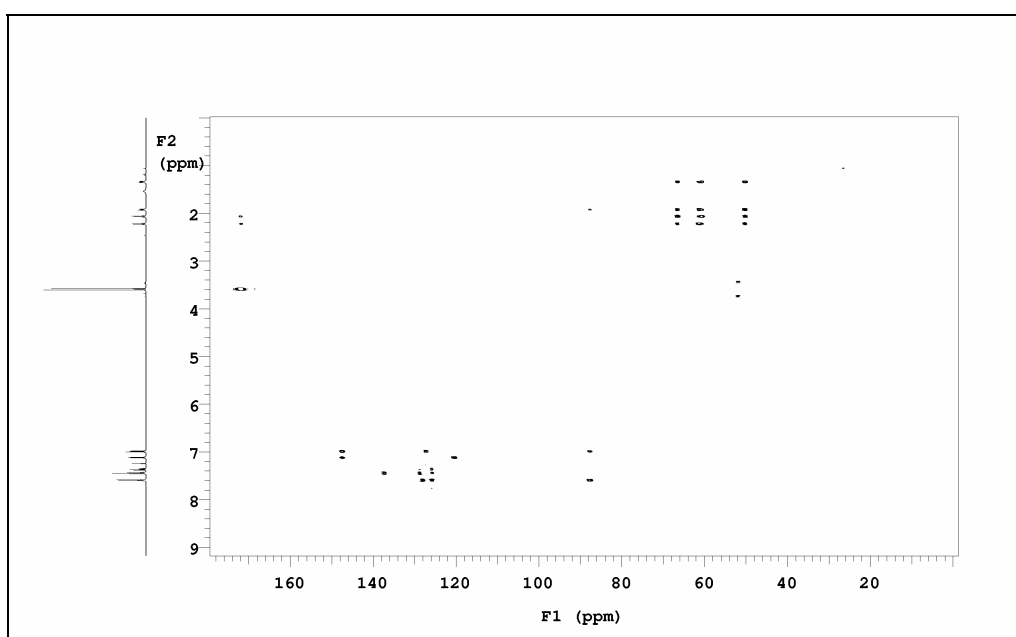


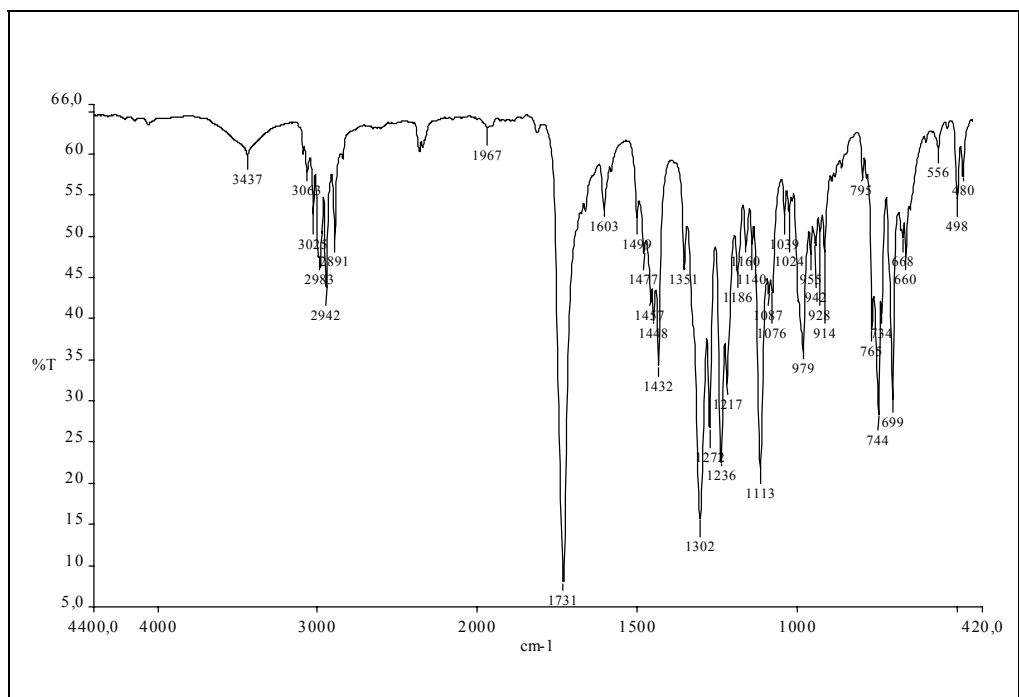
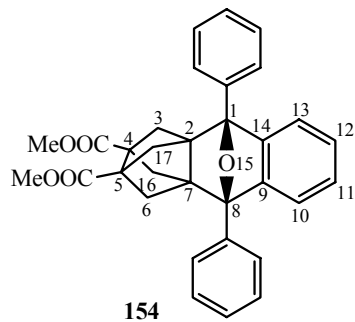


^1H - ^1H -NOESY

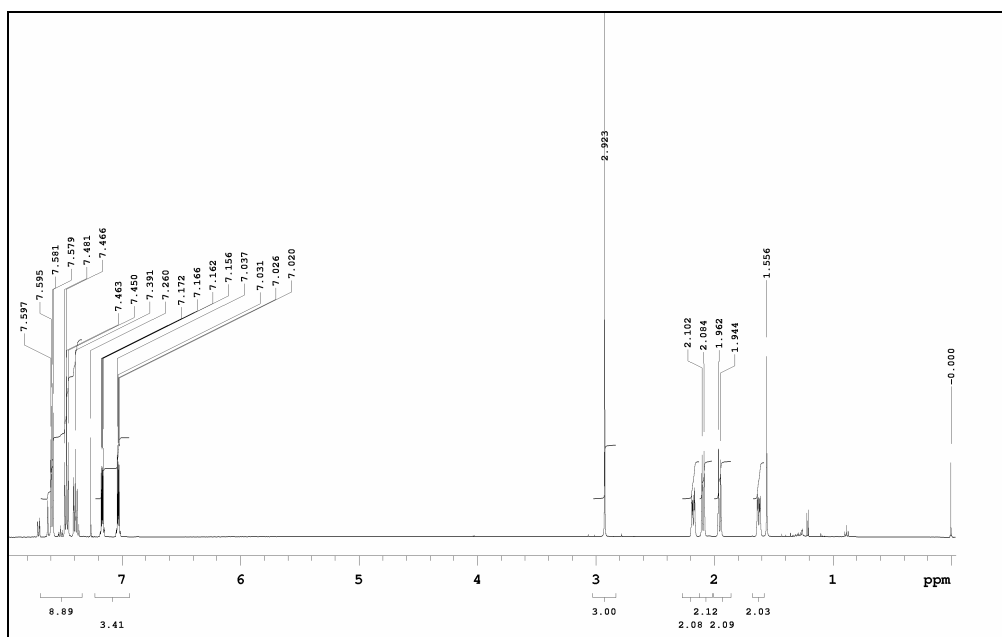
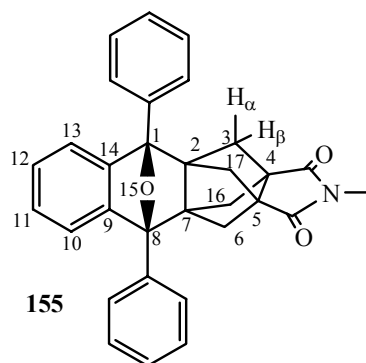


^1H - ^{13}C -HSQC

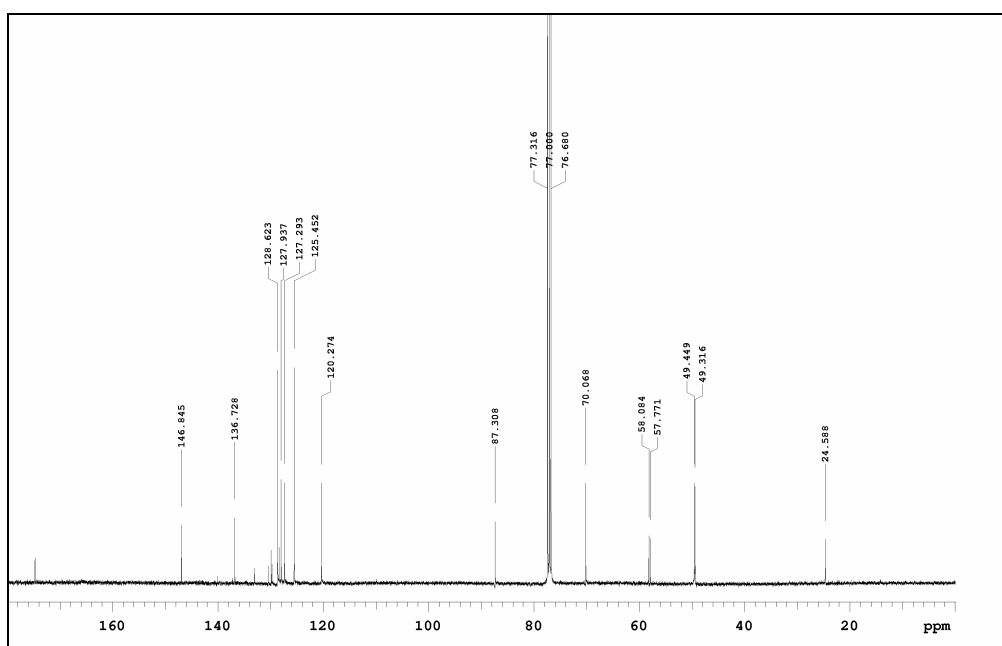
 $^1\text{H}-^{13}\text{C}\text{-HMBC } J = 8 \text{ Hz}$  $^1\text{H}-^{13}\text{C}\text{-HMBC } J = 5 \text{ Hz}$



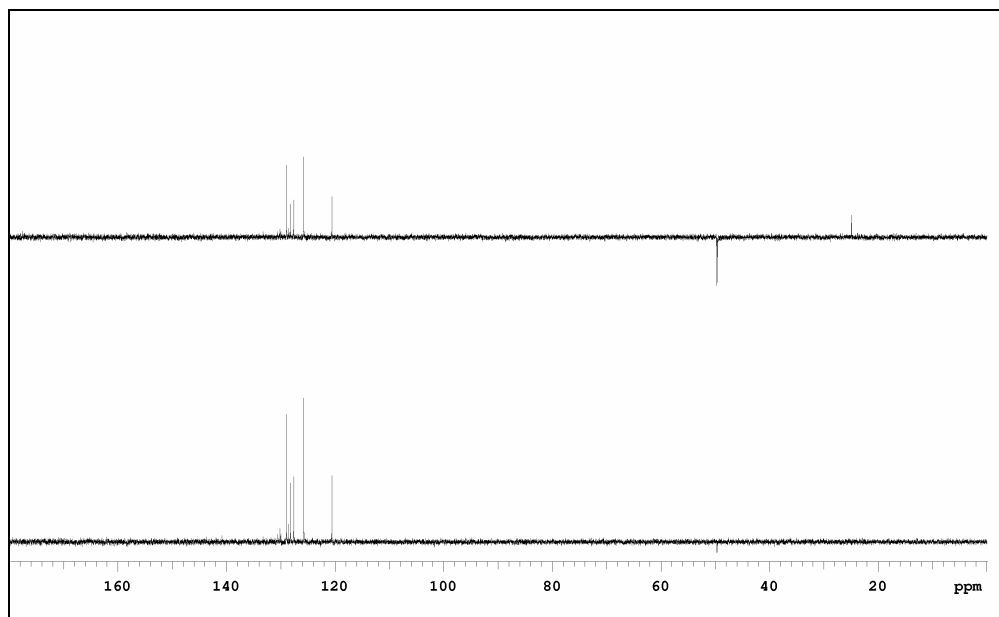
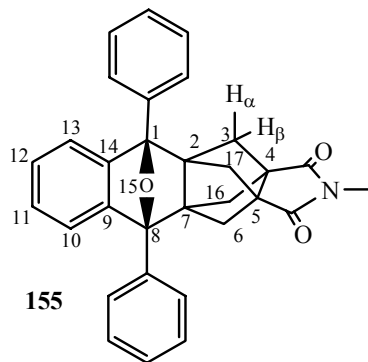
IR (KBr)



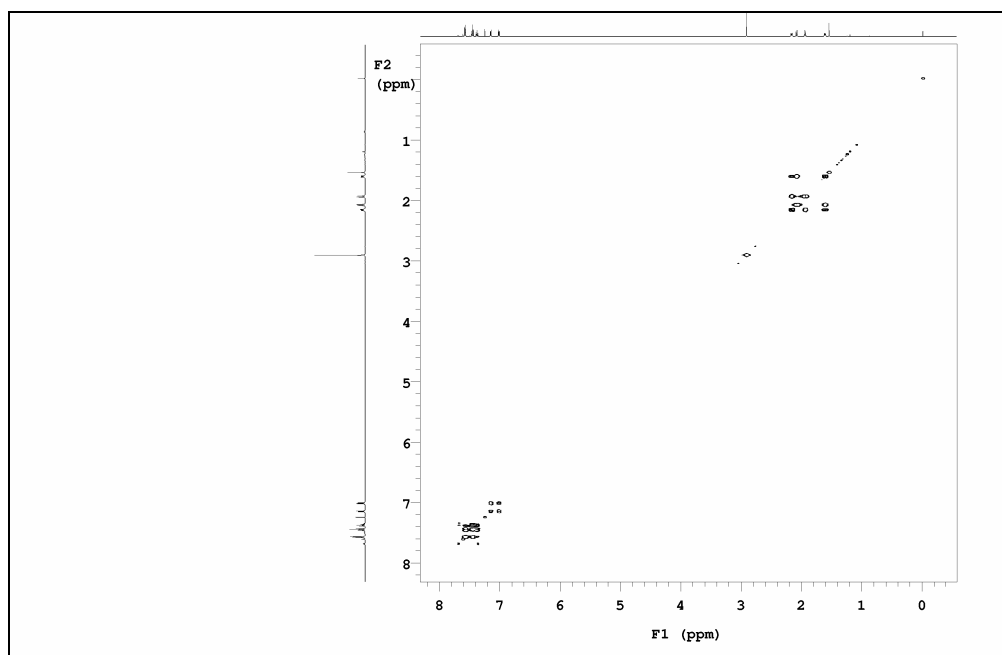
$^1\text{H-RMN}$ (500 MHz, CDCl_3)



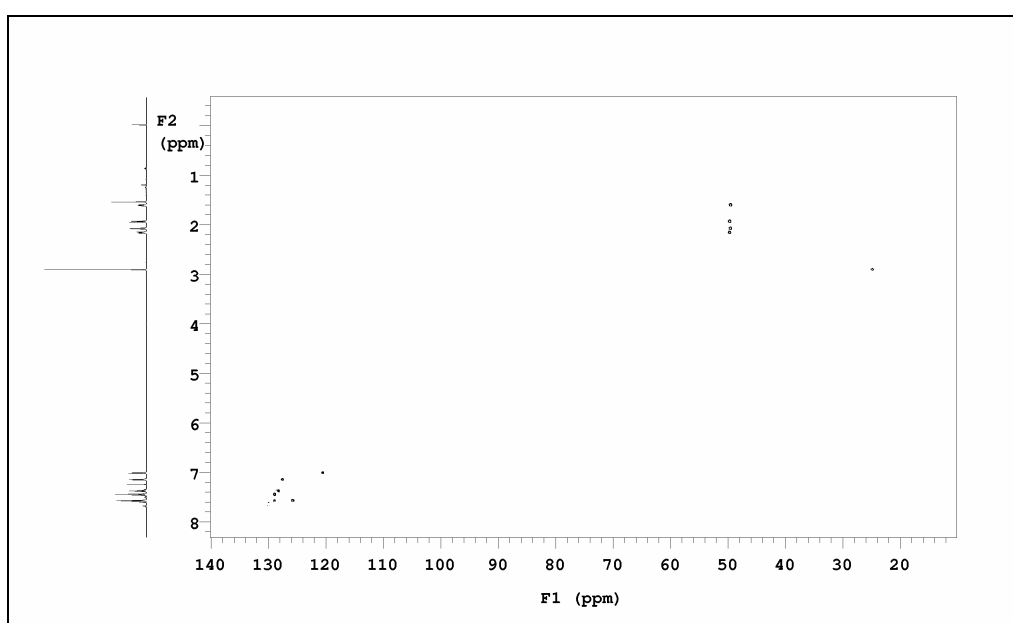
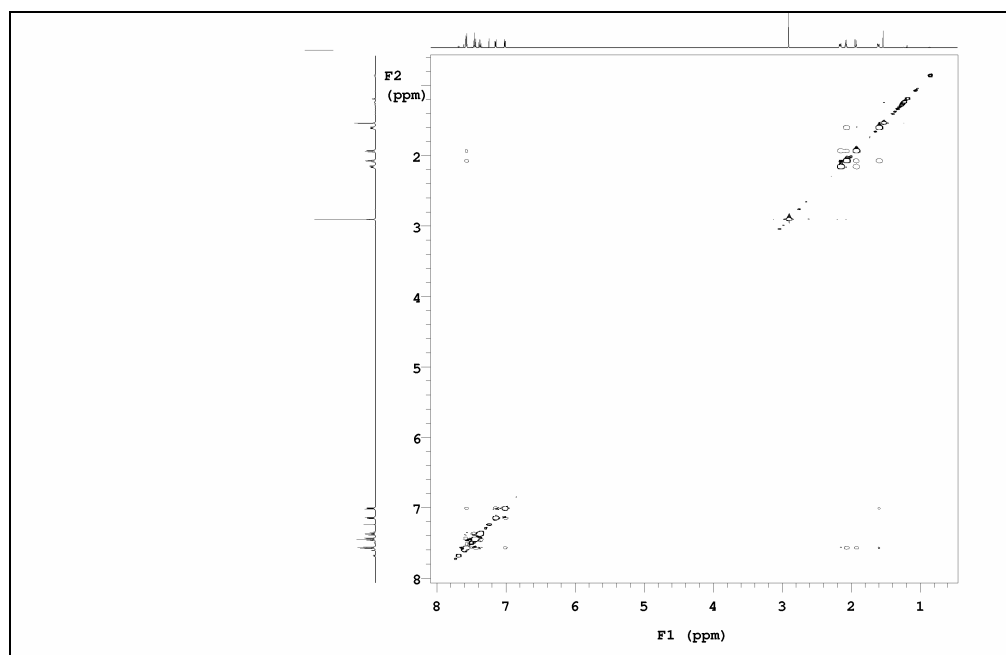
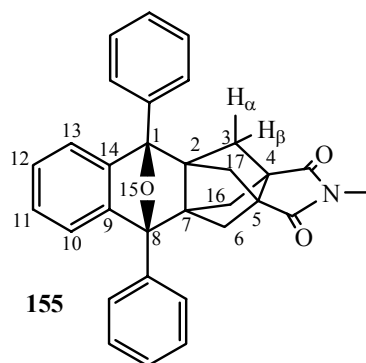
$^{13}\text{C-RMN}$ (100.6 MHz, CDCl_3)

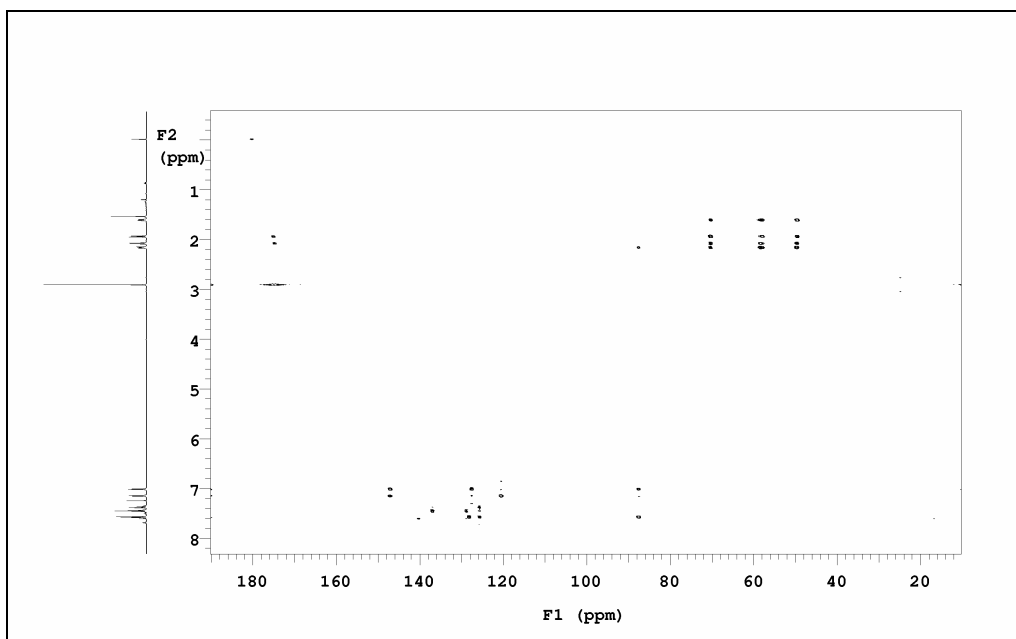
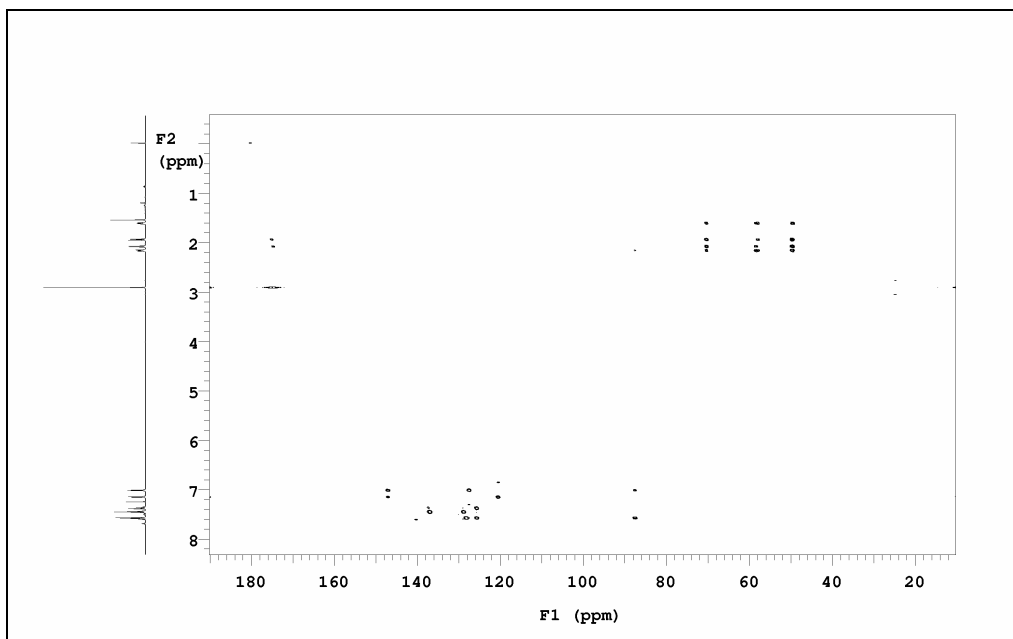
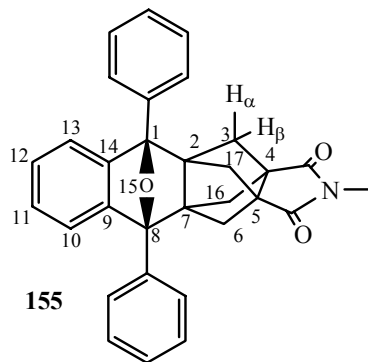


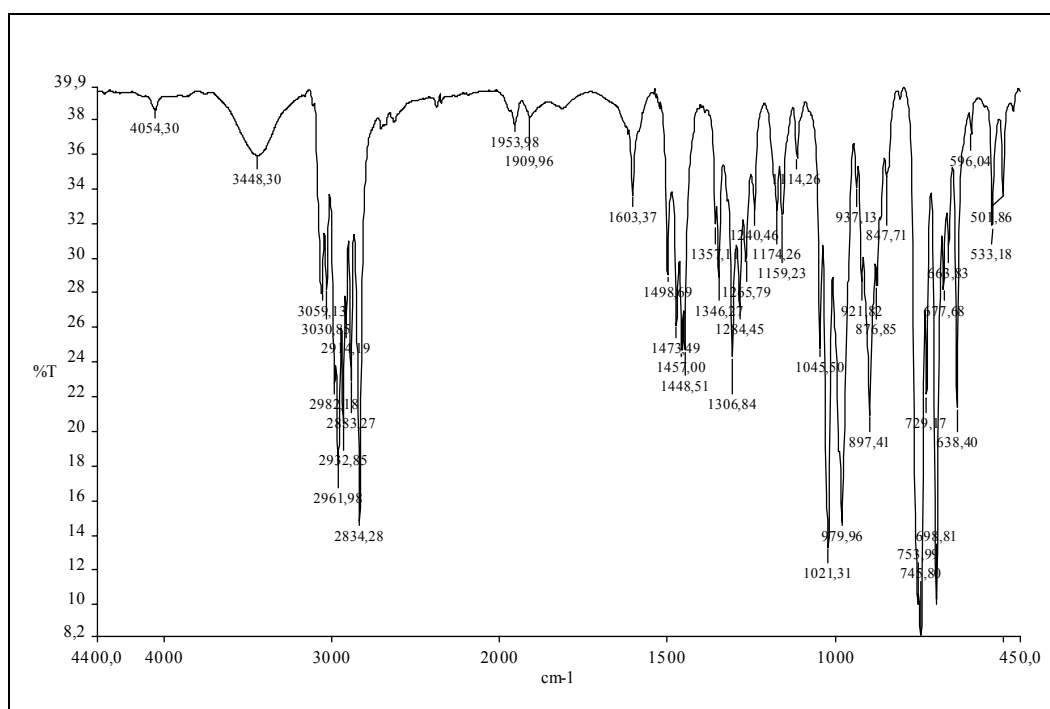
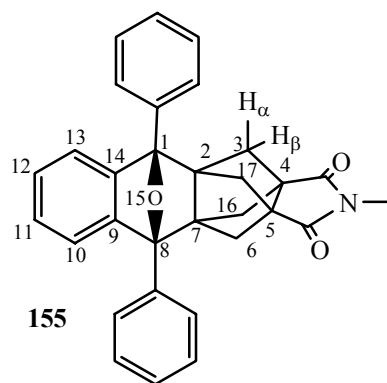
$^{13}\text{C-DEPT}$



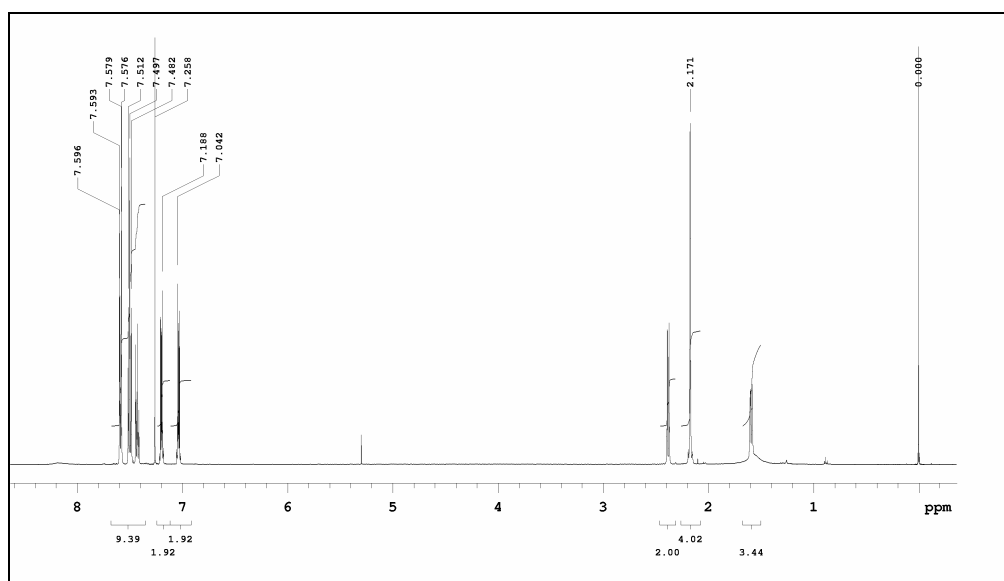
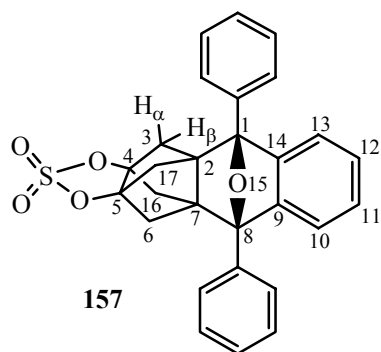
$^1\text{H-}^1\text{H-COSY}$



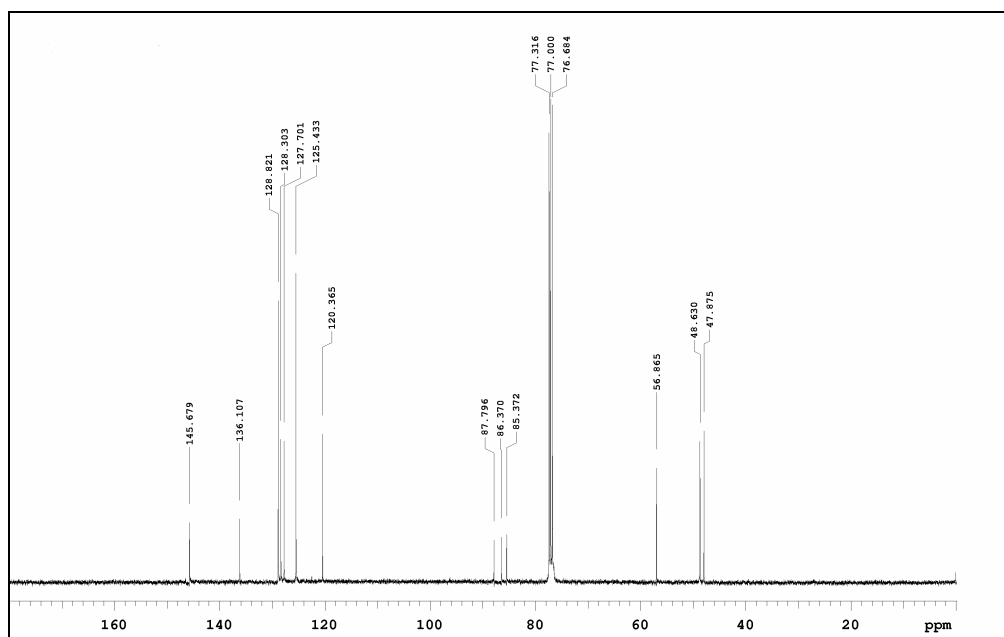




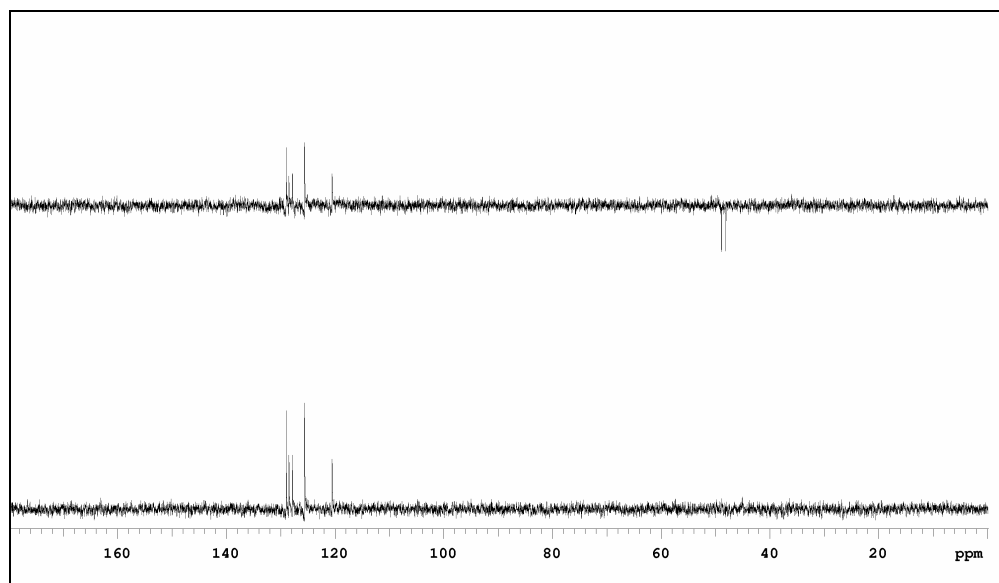
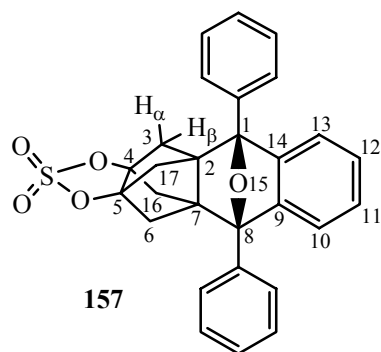
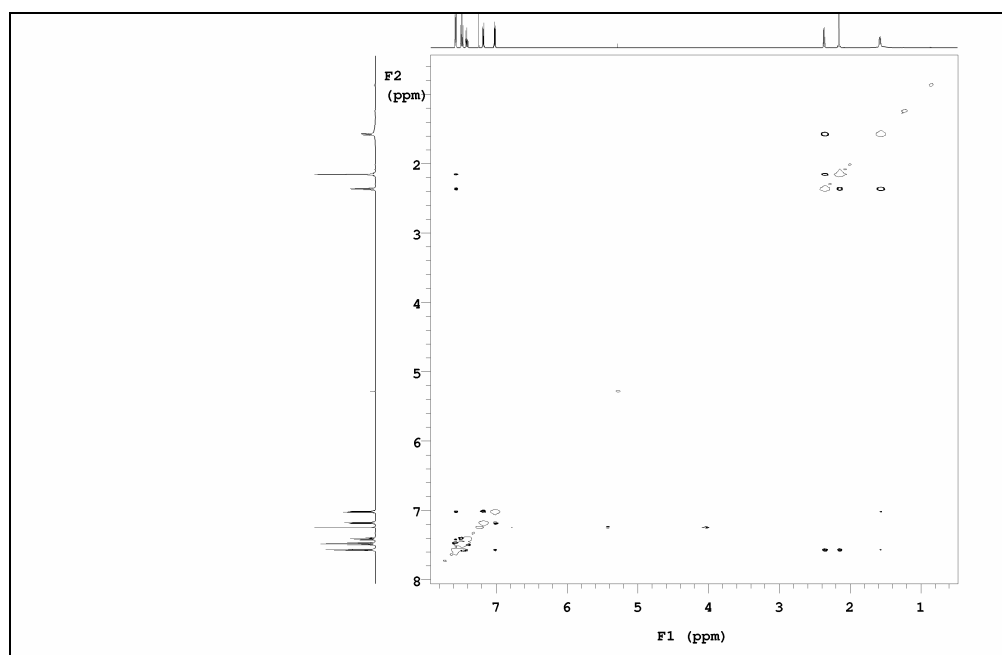
IR (KBr)

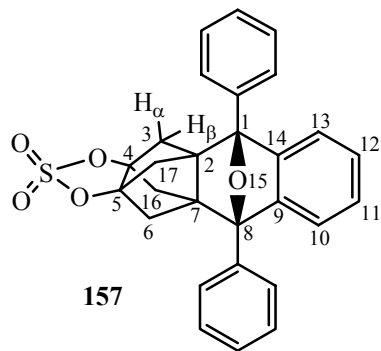


$^1\text{H-RMN}$ (500 MHz, CDCl_3)

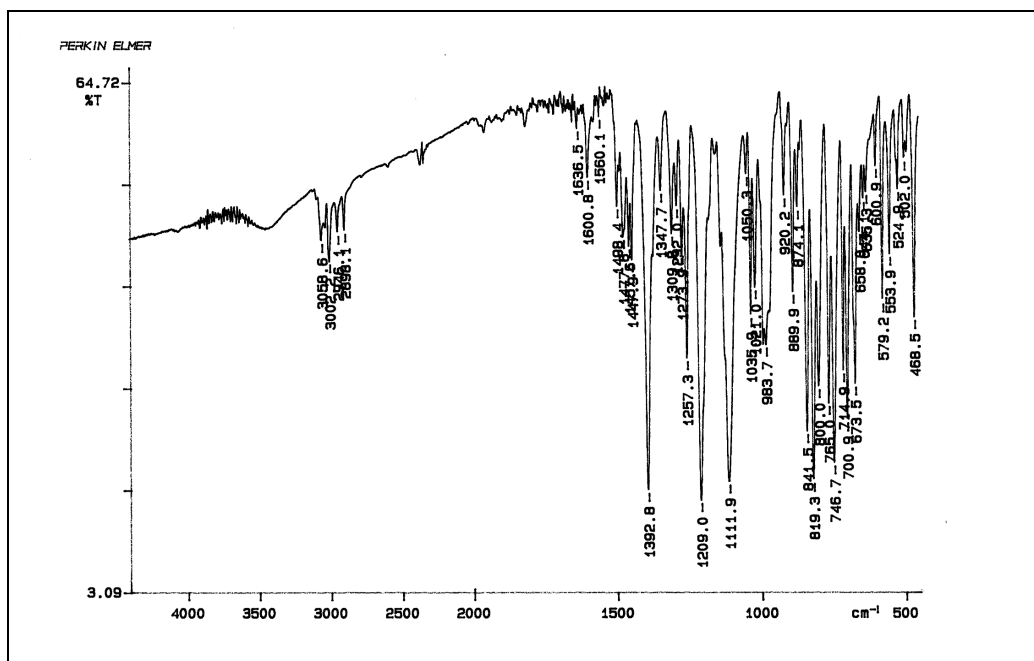


$^{13}\text{C-RMN}$ (100.6 MHz, CDCl_3)

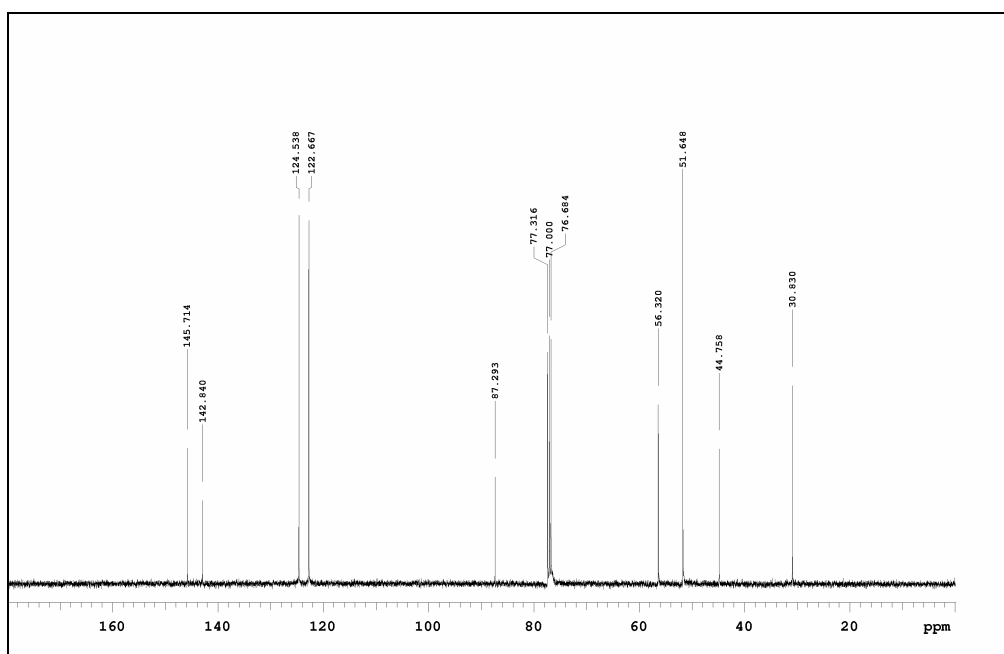
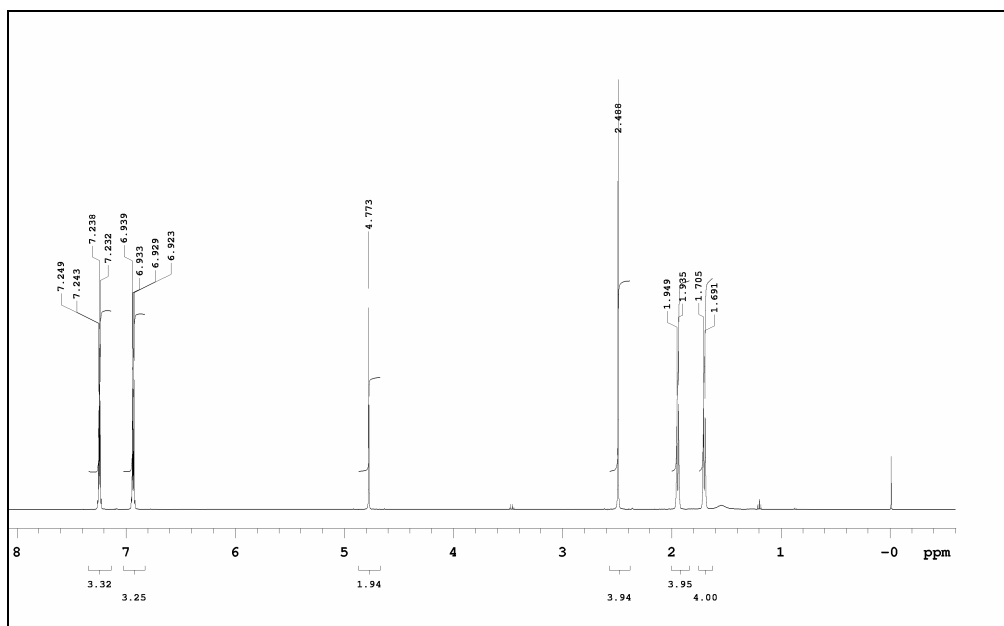
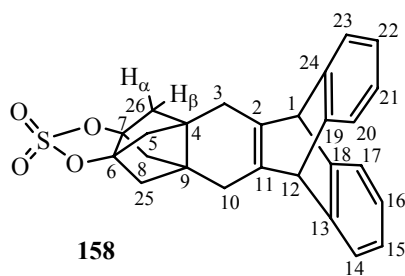
 ^{13}C -DEPT ^1H - ^1H -NOESY

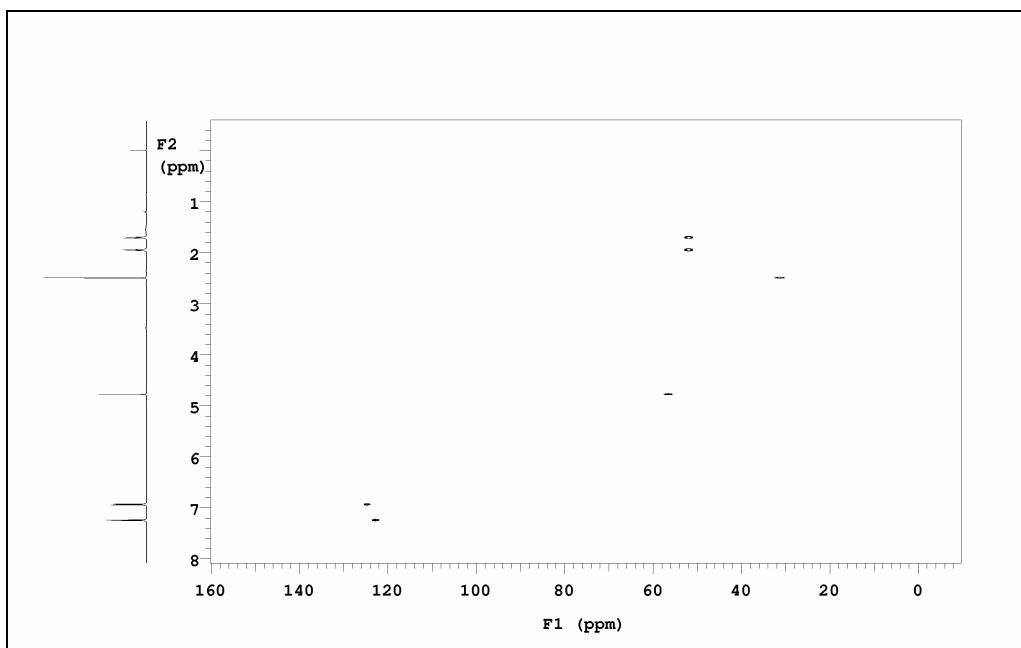
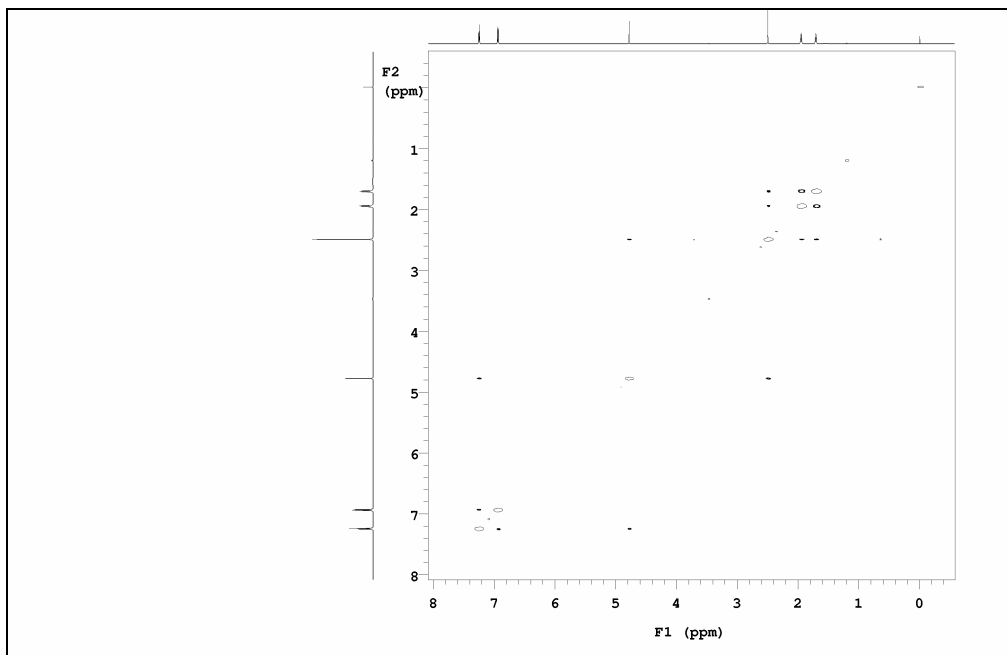
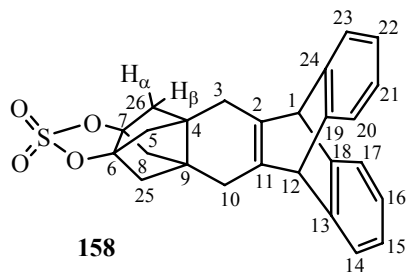


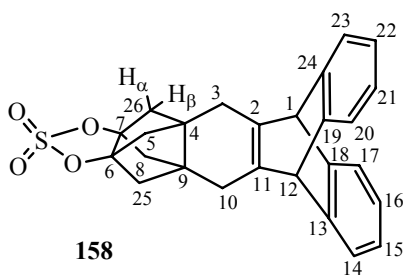
157



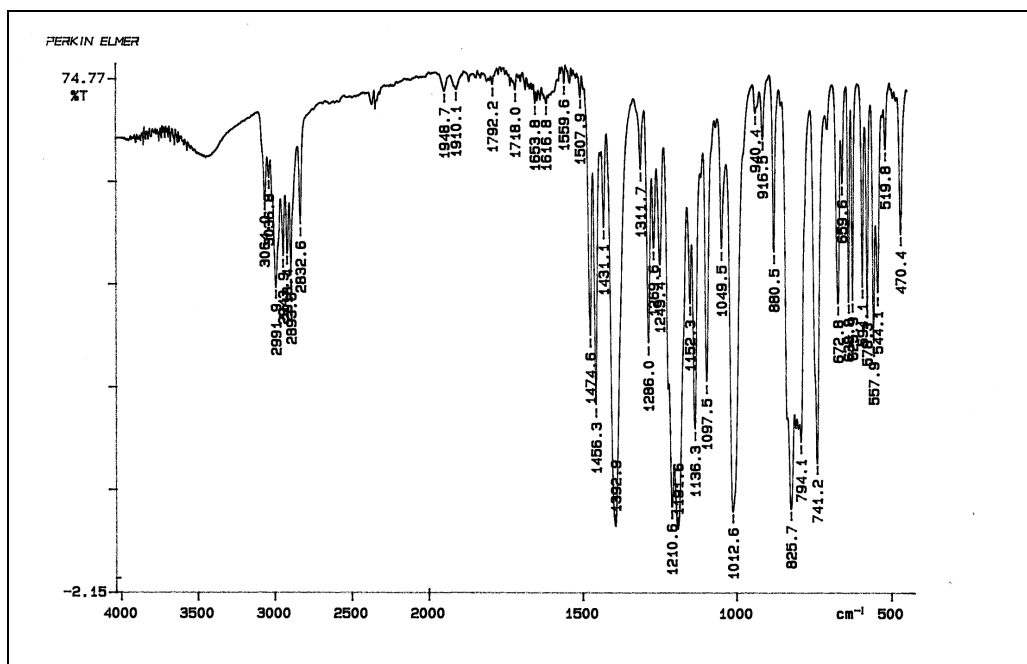
IR (KBr)



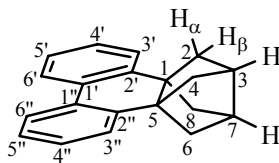




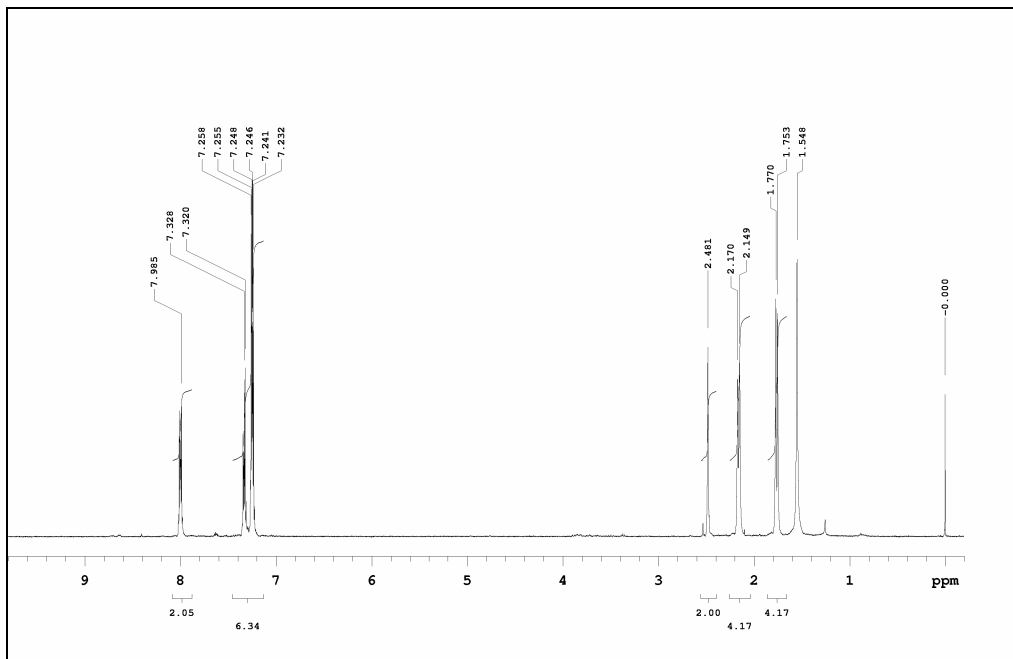
158



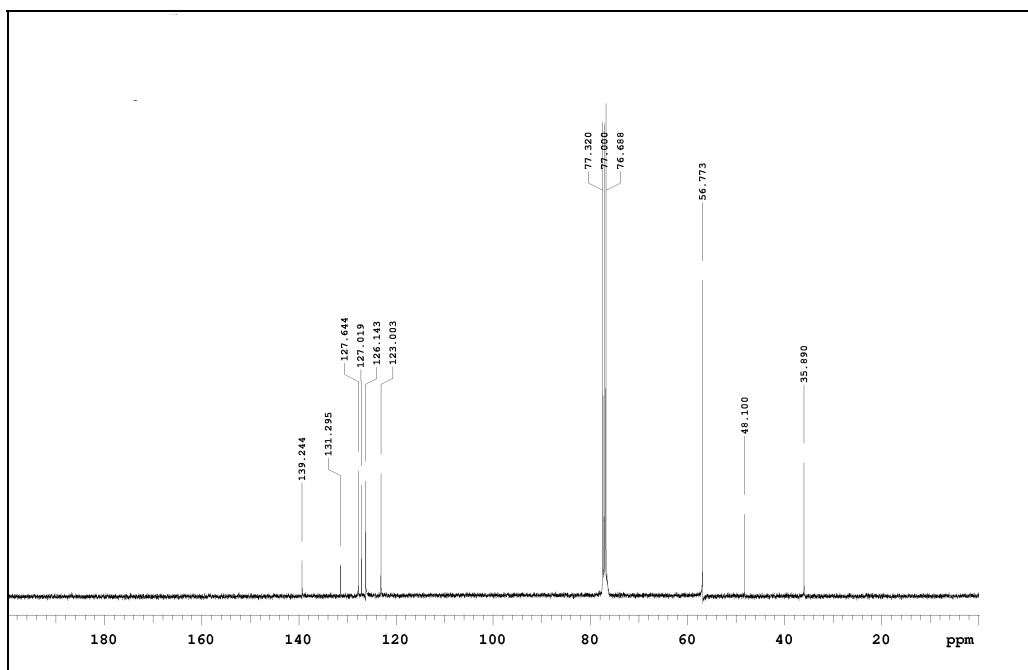
IR (KBr)



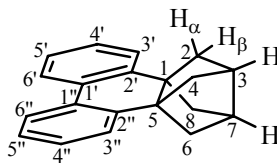
162



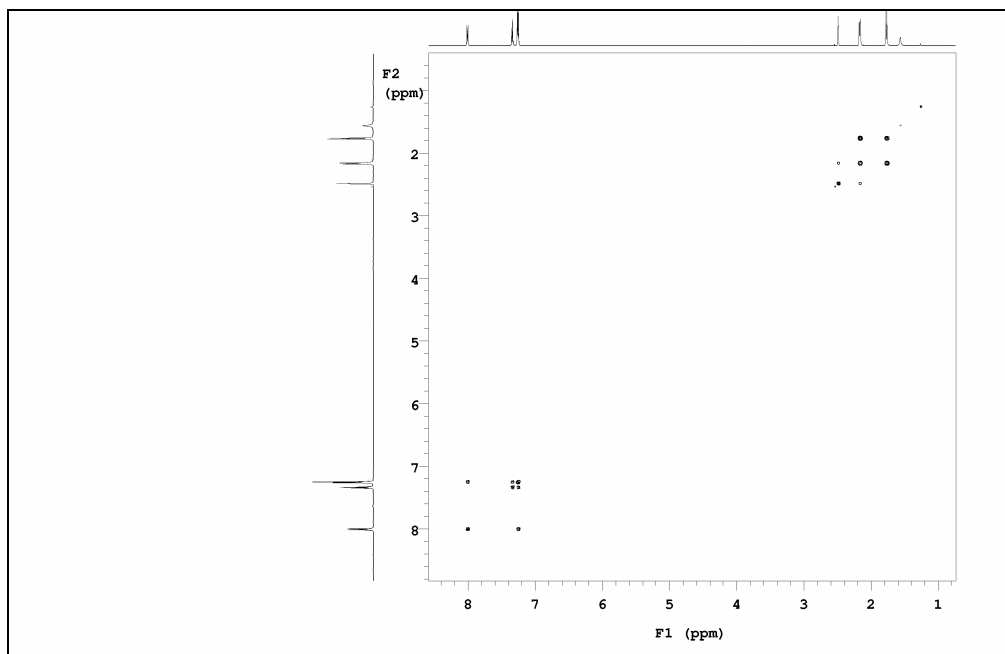
¹H-RMN (500 MHz, CDCl₃)



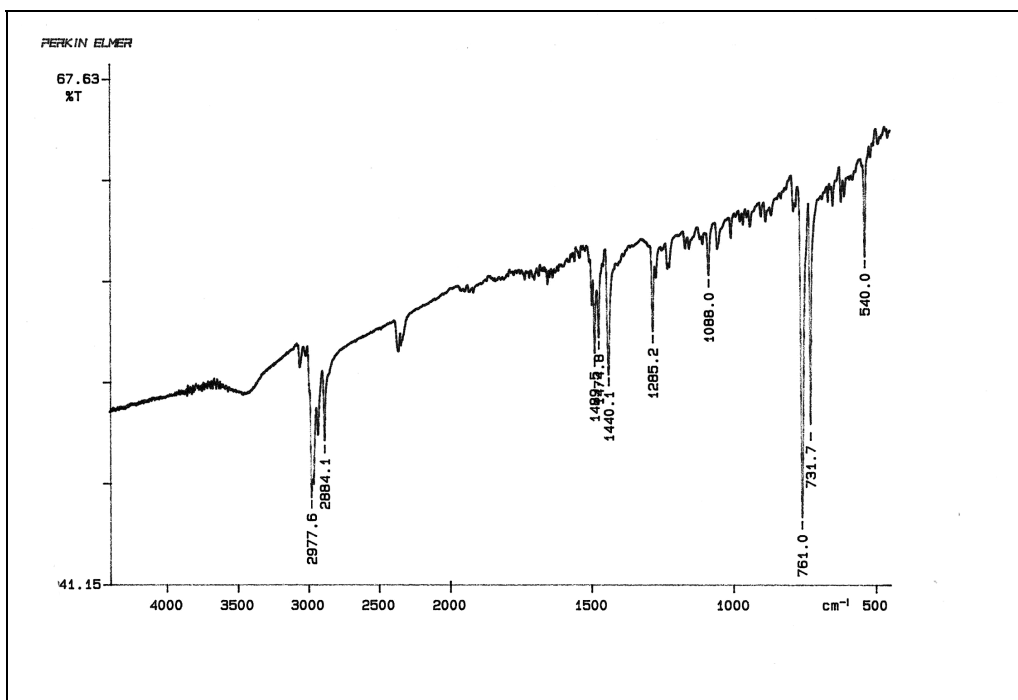
¹³C-RMN (100.6 MHz, CDCl₃)



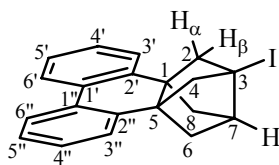
162



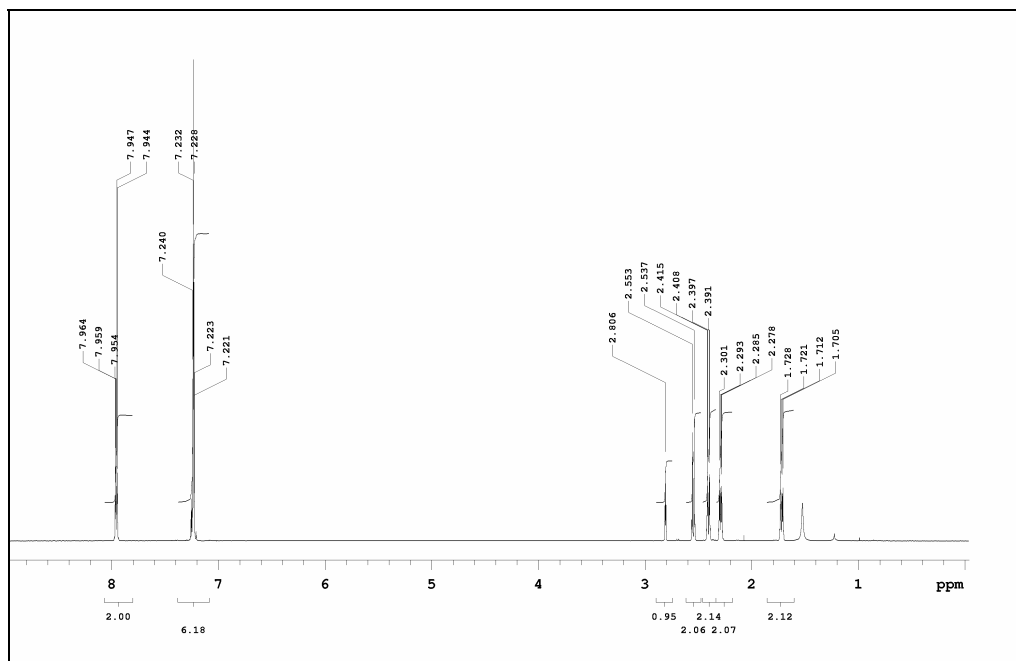
¹H-¹H-COSY



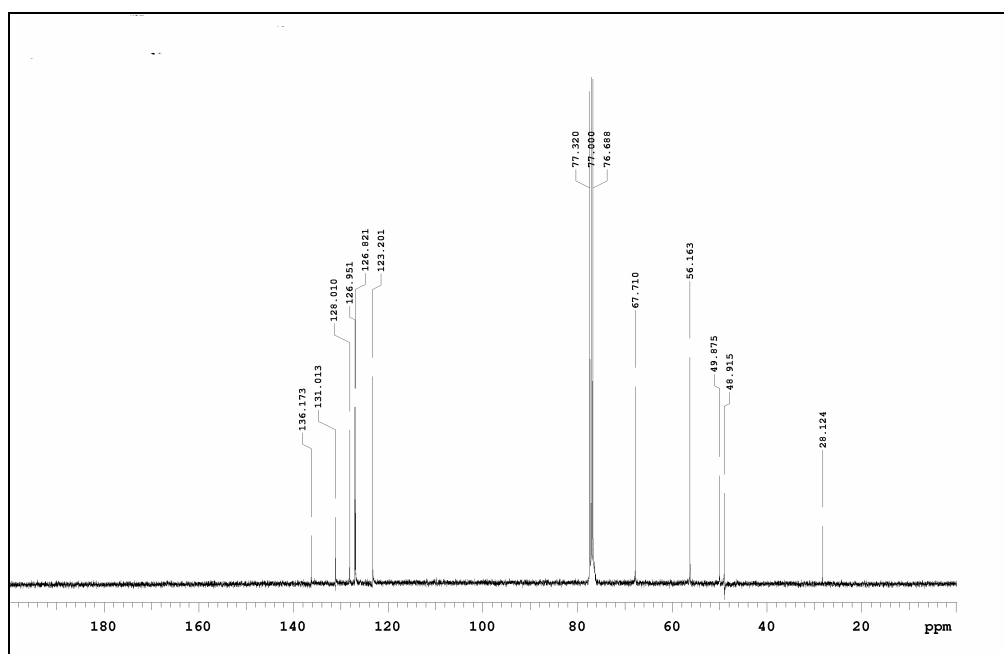
IR (KBr)



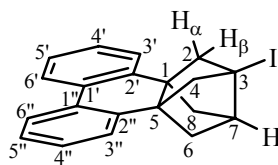
167



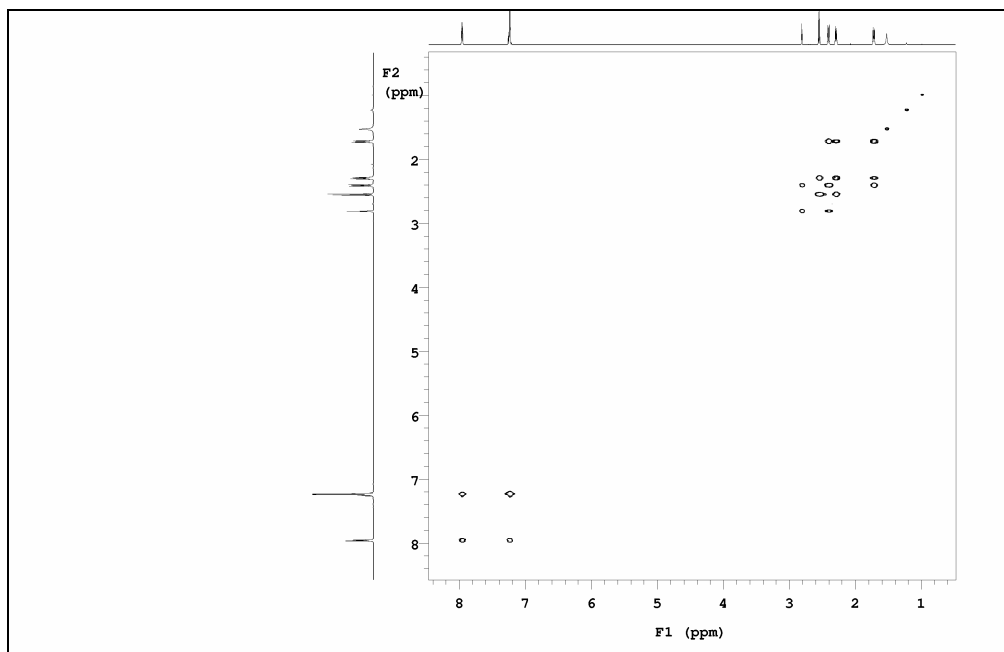
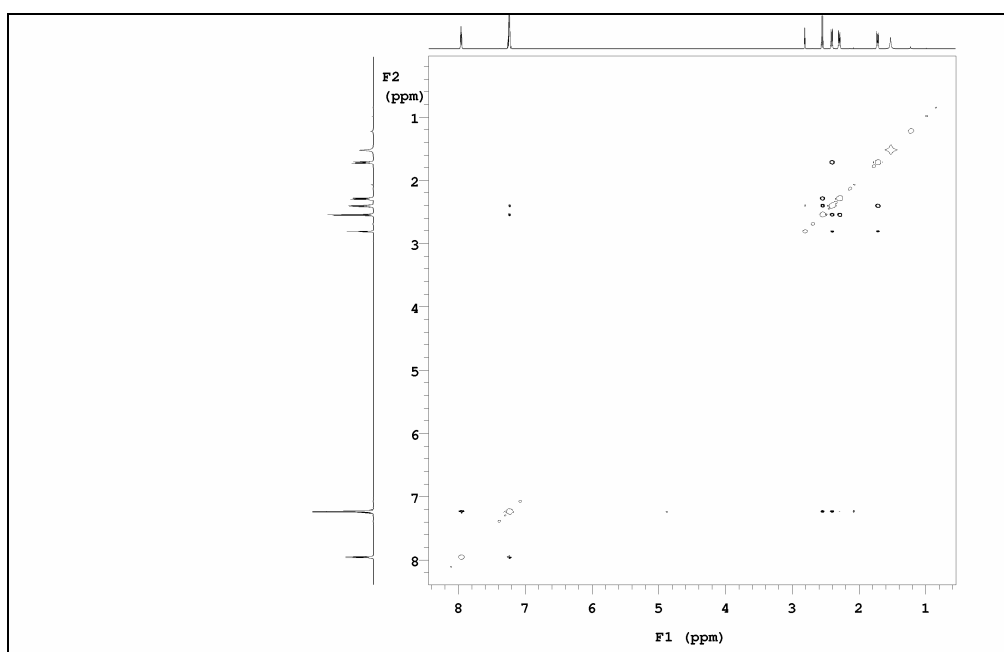
$^1\text{H-RMN}$ (500 MHz, CDCl_3)

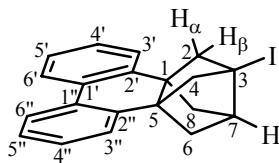


$^{13}\text{C-RMN}$ (100.6 MHz, CDCl_3)

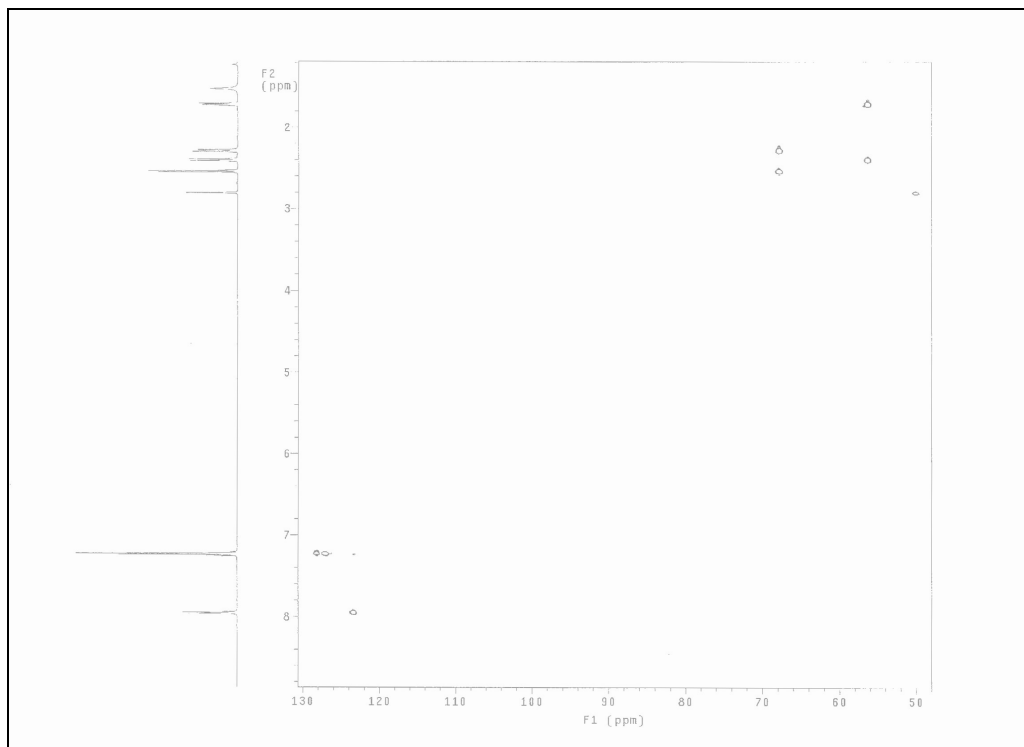


167

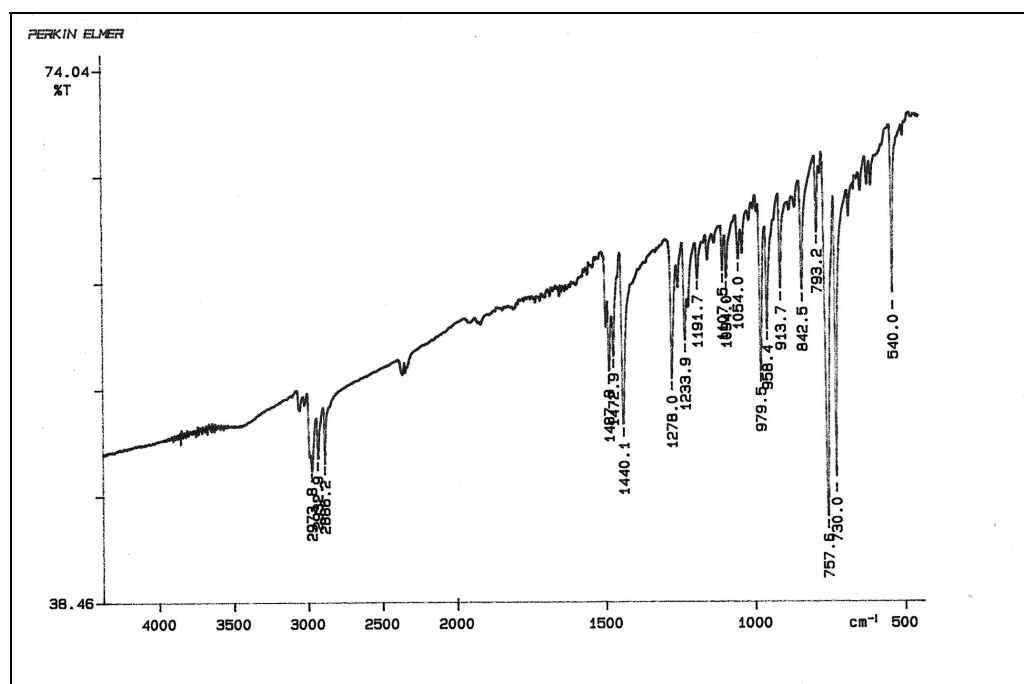
 ^1H - ^1H -COSY ^1H - ^1H -NOESY



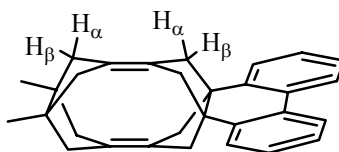
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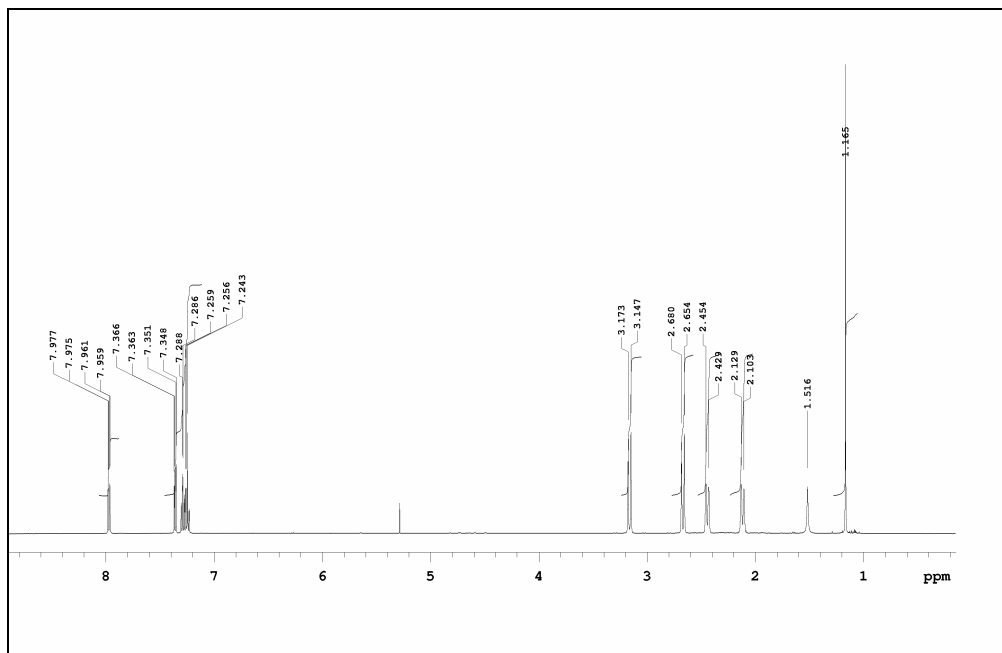
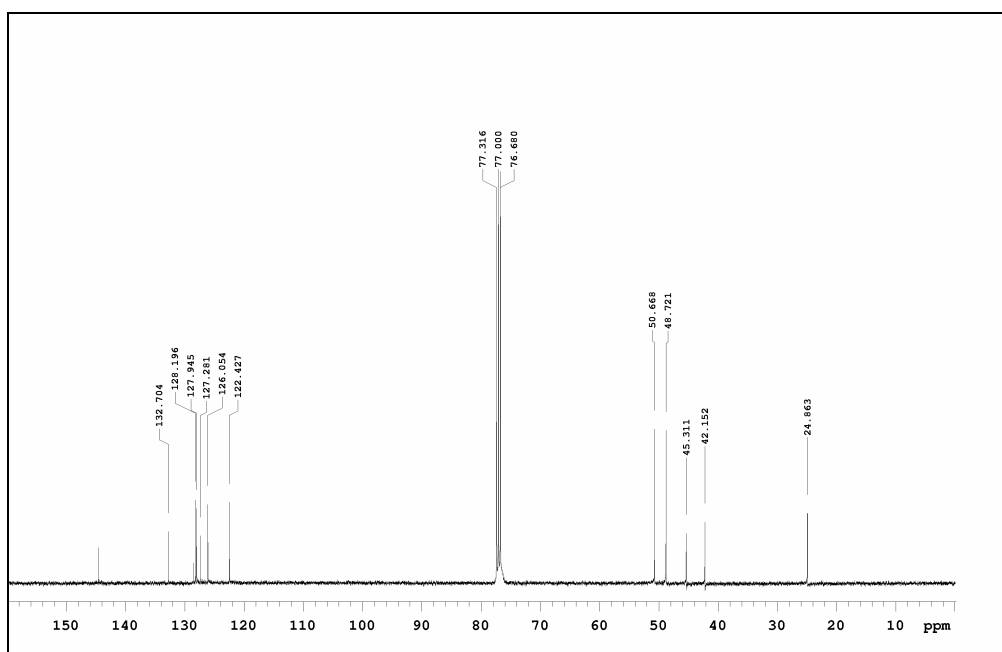
$^1\text{H}-^{13}\text{C}$ -HSQC

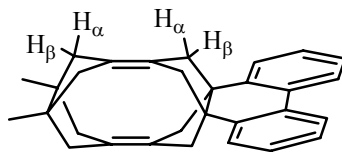


IR (KBr)

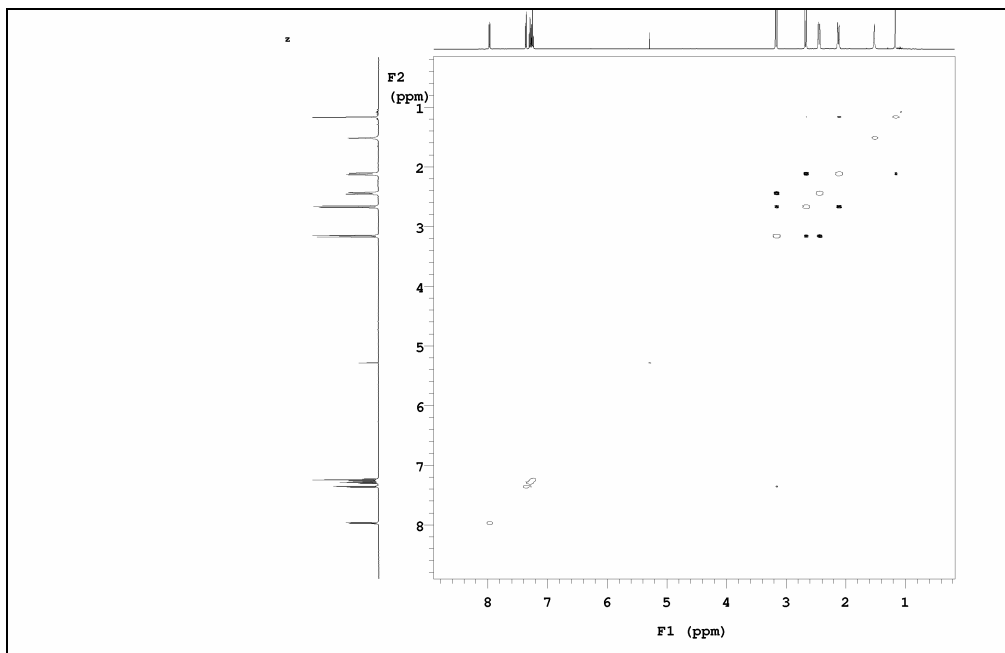


177

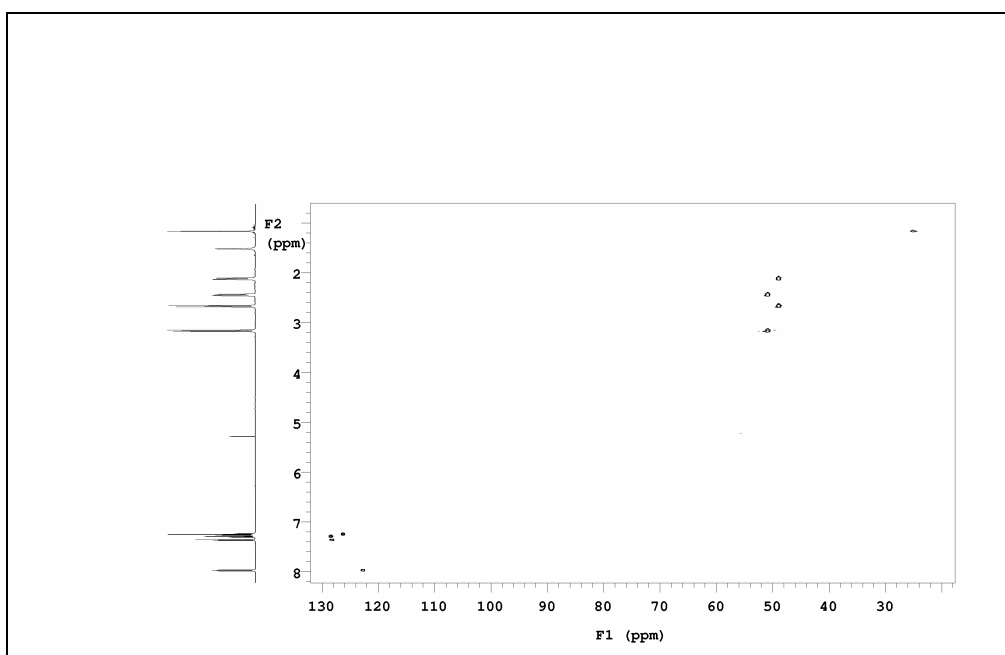
 $^1\text{H-RMN}$ (500 MHz, CDCl_3) $^{13}\text{C-RMN}$ (100.6 MHz, CDCl_3)



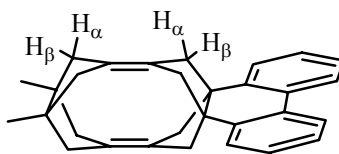
177



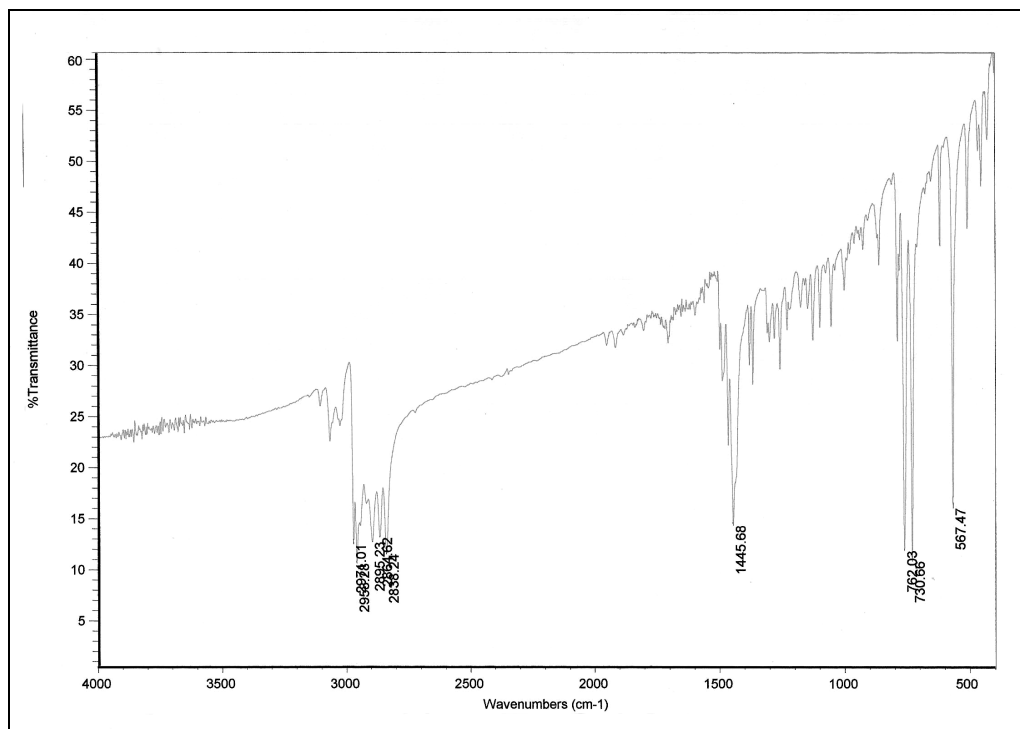
¹H-¹H-NOESY



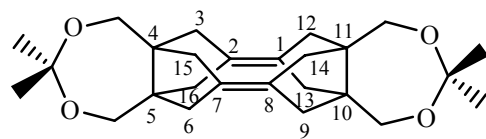
¹H-¹³C-HSQC



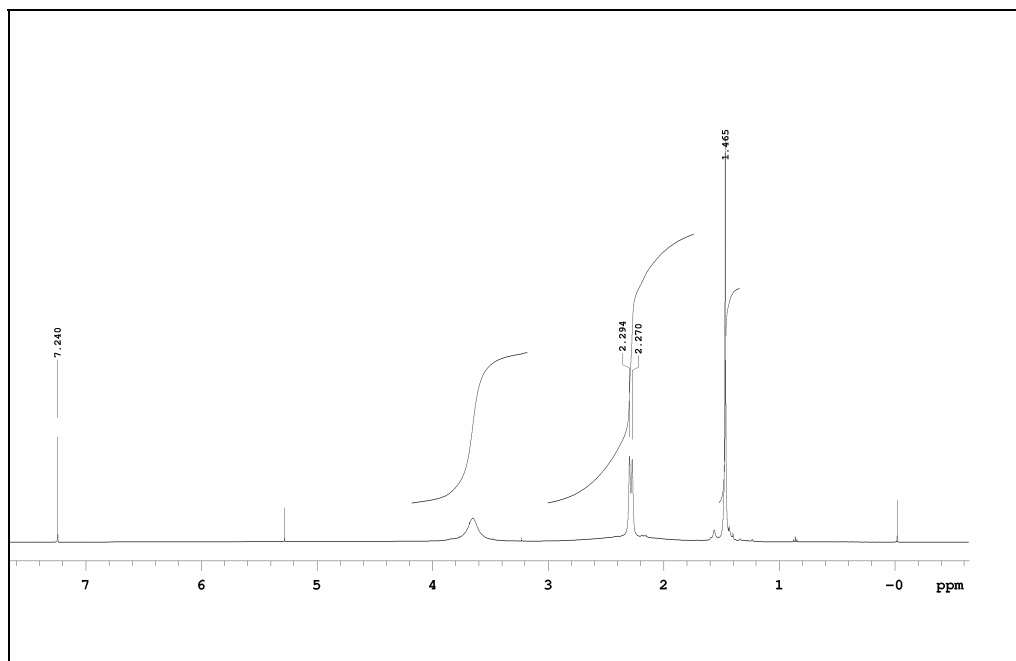
177



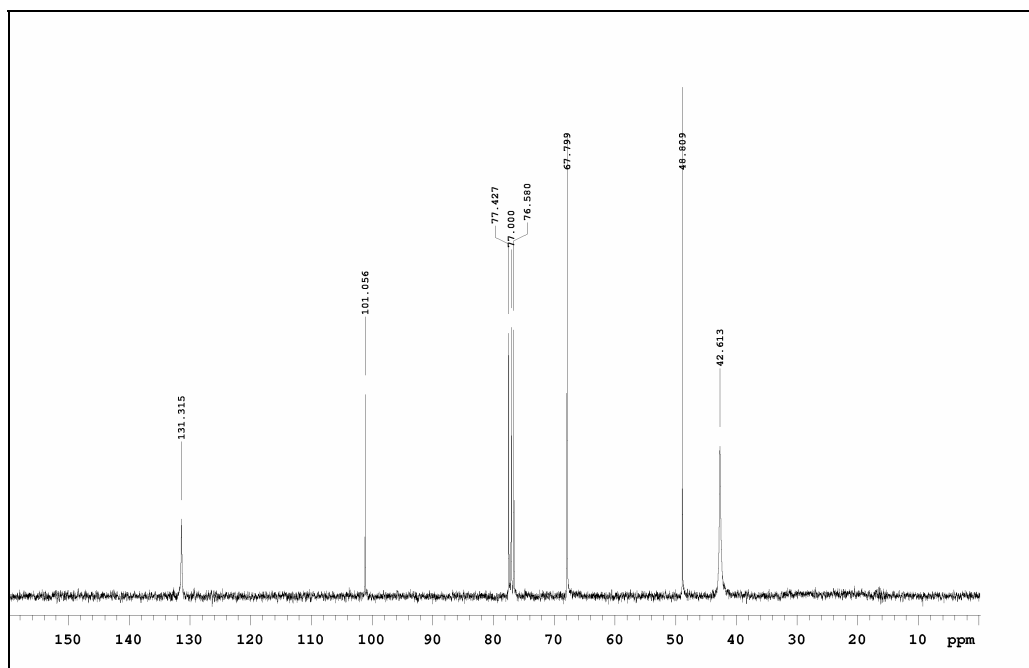
IR (KBr)



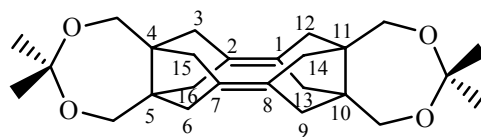
180



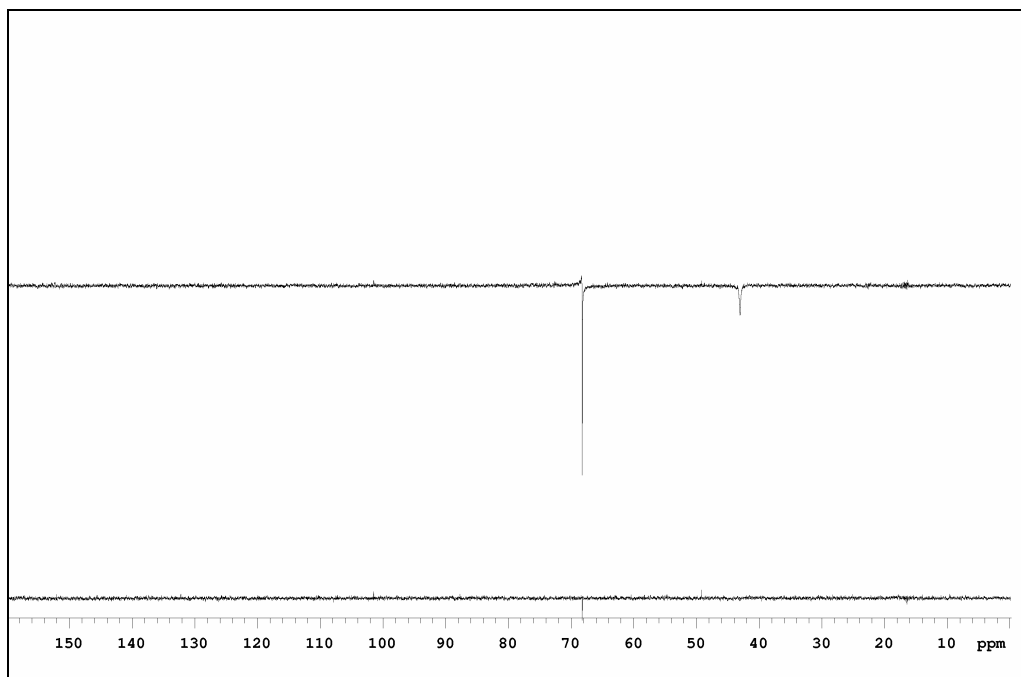
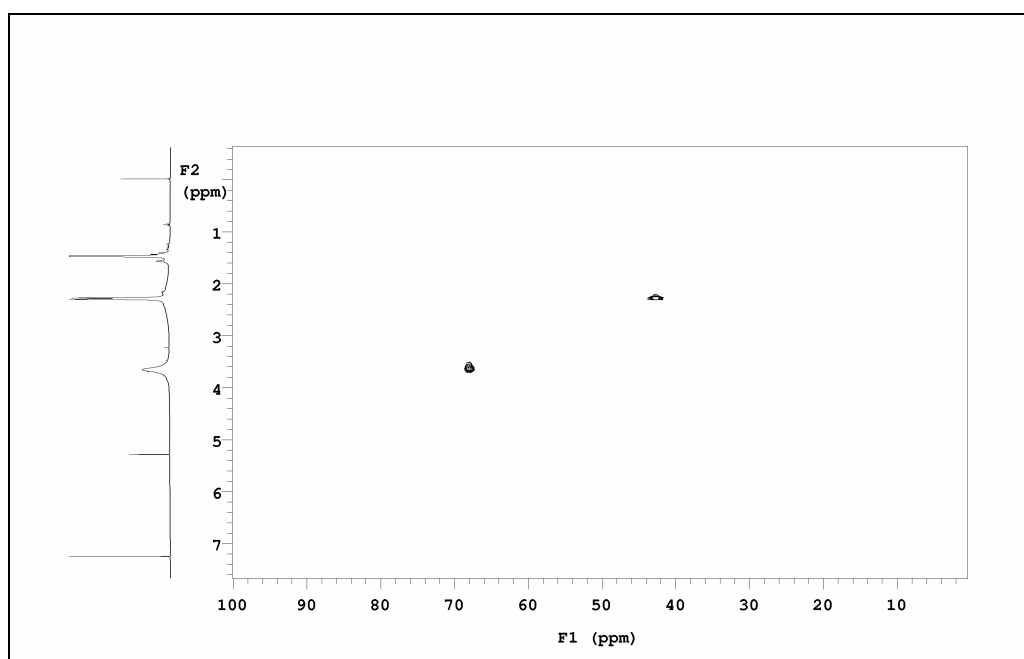
$^1\text{H-RMN}$ (500 MHz, CDCl_3) a 25°C

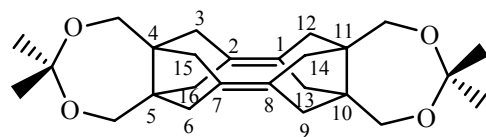


$^{13}\text{C-RMN}$ (75.4 MHz, CDCl_3)

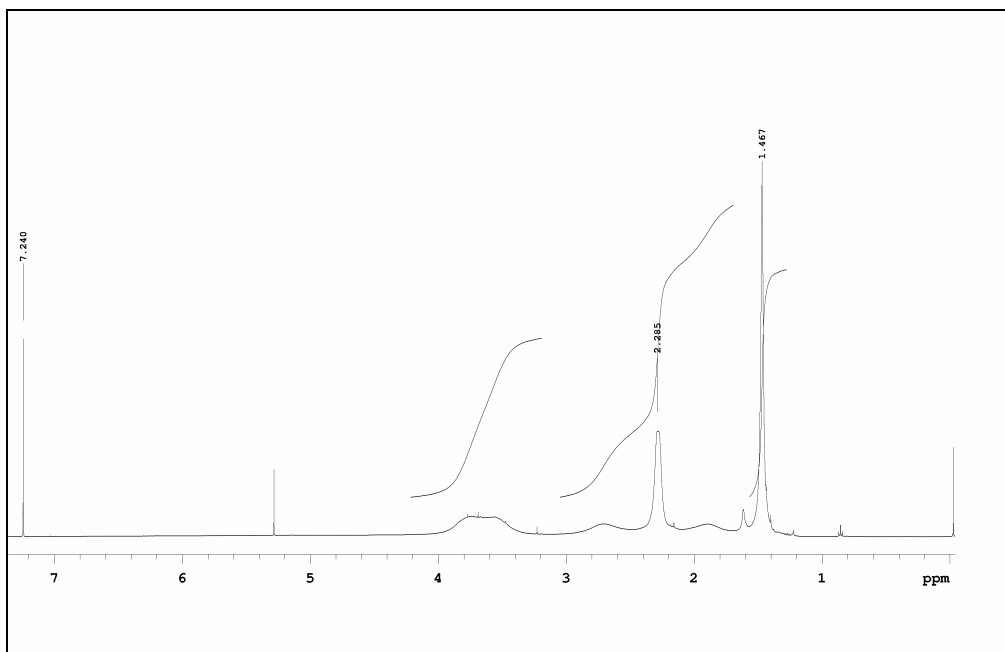


180

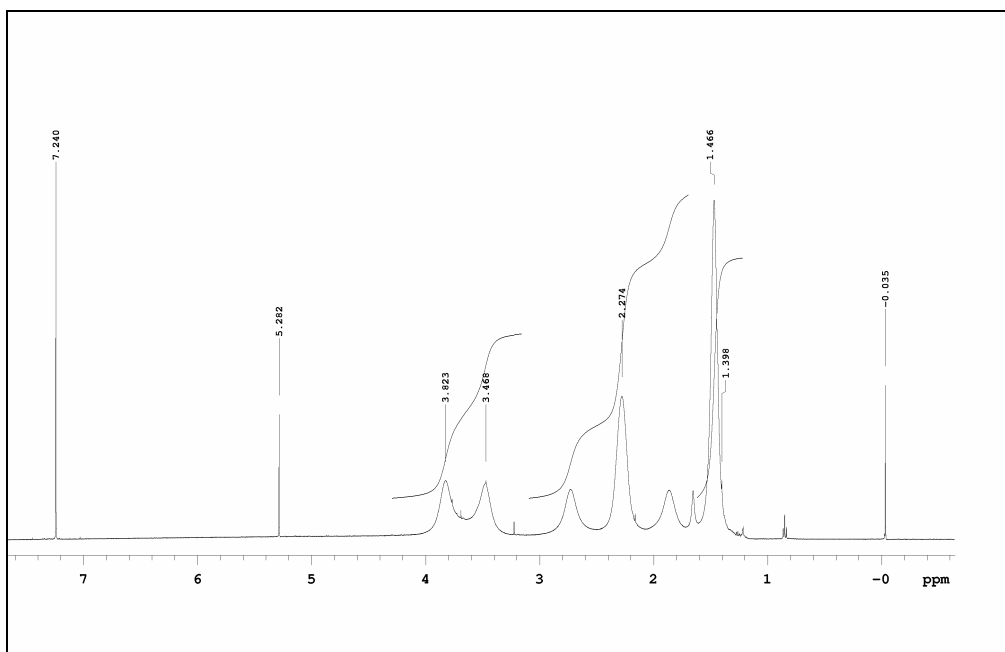
 ^{13}C -DEPT ^1H - ^{13}C -HSQC a 25°C



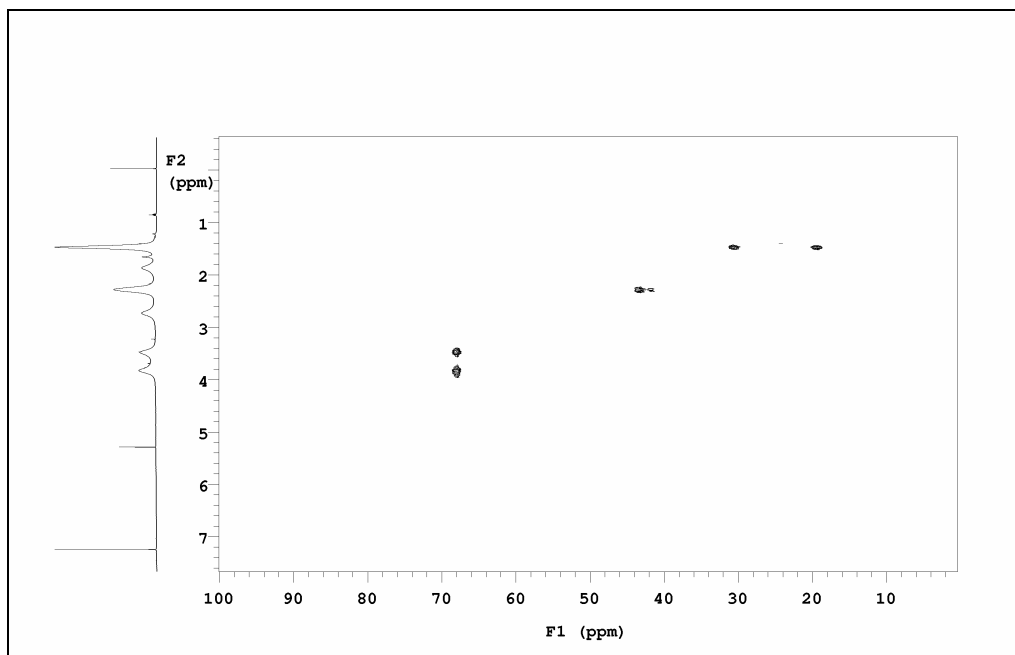
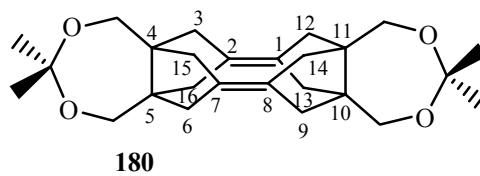
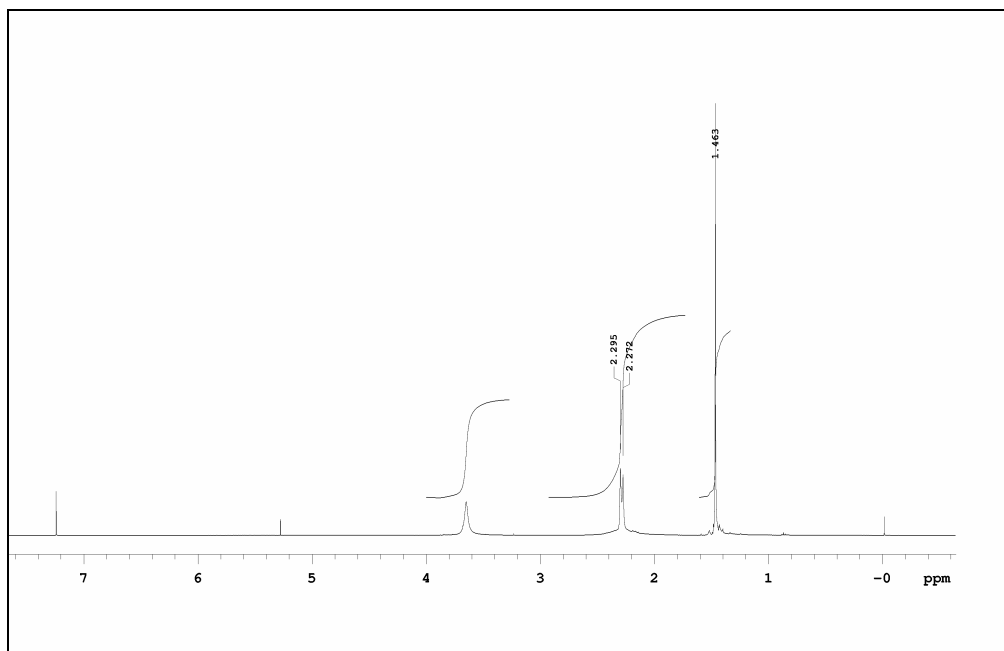
180

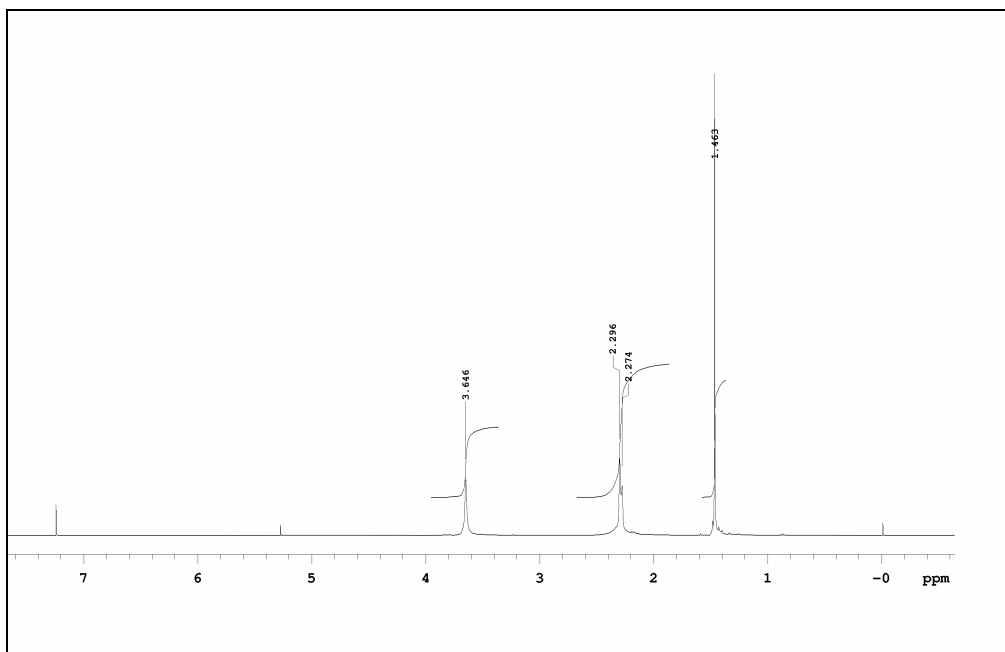
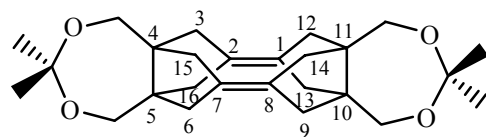


$^1\text{H-RMN}$ (500 MHz, CDCl_3) a 10°C

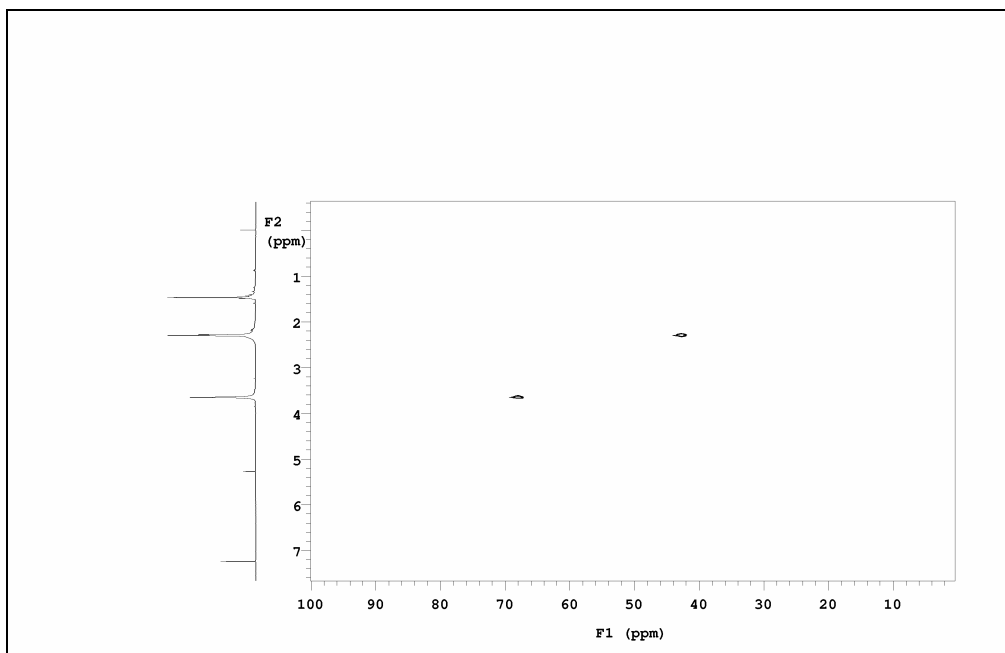


$^1\text{H-RMN}$ (500 MHz, CDCl_3) a 0°C

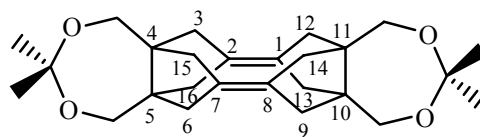
 $^1\text{H}-^{13}\text{C}$ -HSQC a 0°C ^1H -RMN (500 MHz, CDCl_3) a 40 °C



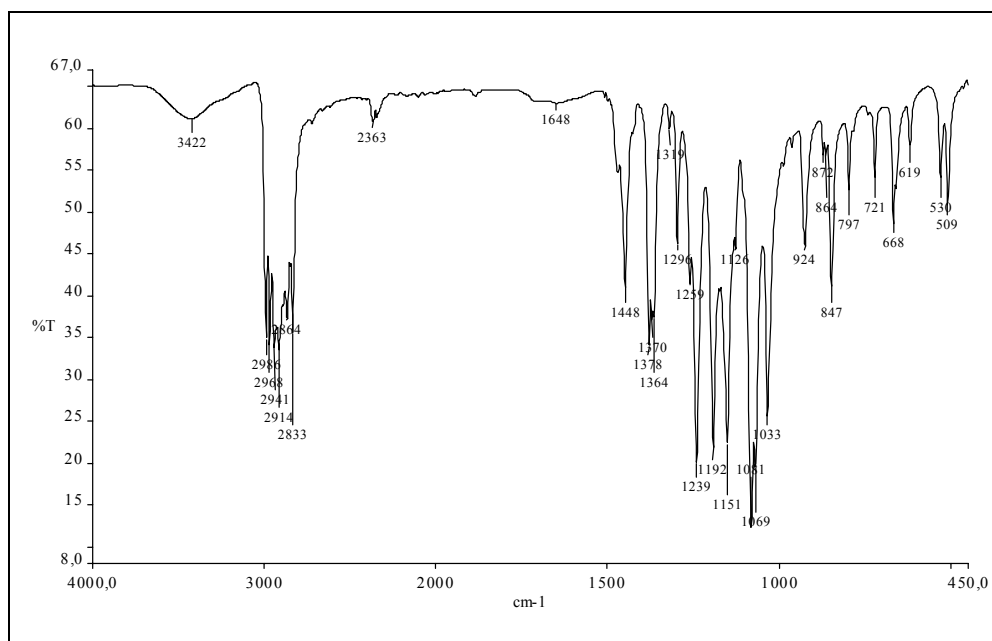
^1H -RMN (500 MHz, CDCl_3) a 50°C



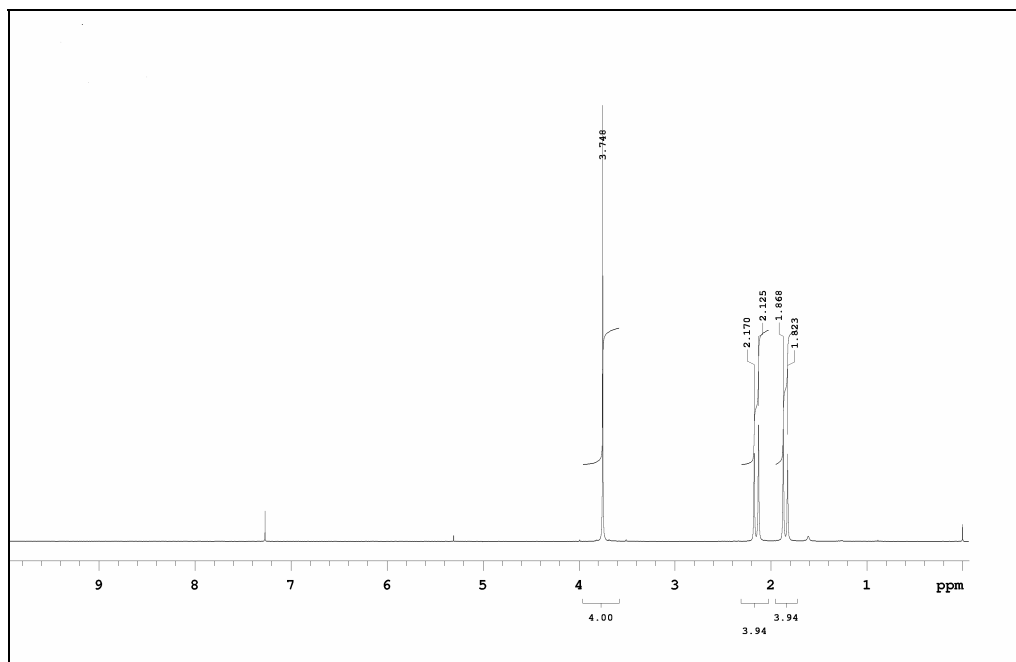
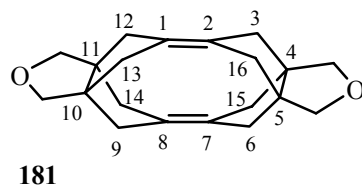
^1H - ^{13}C -HSQC a 50°C



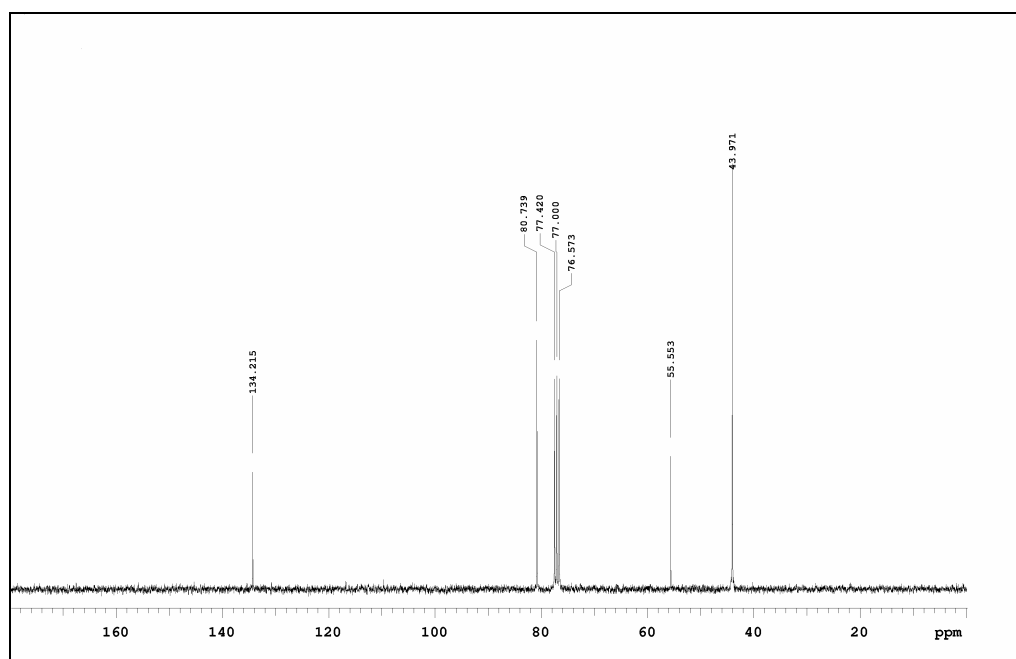
180



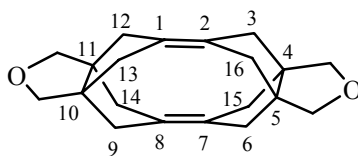
IR (KBr)



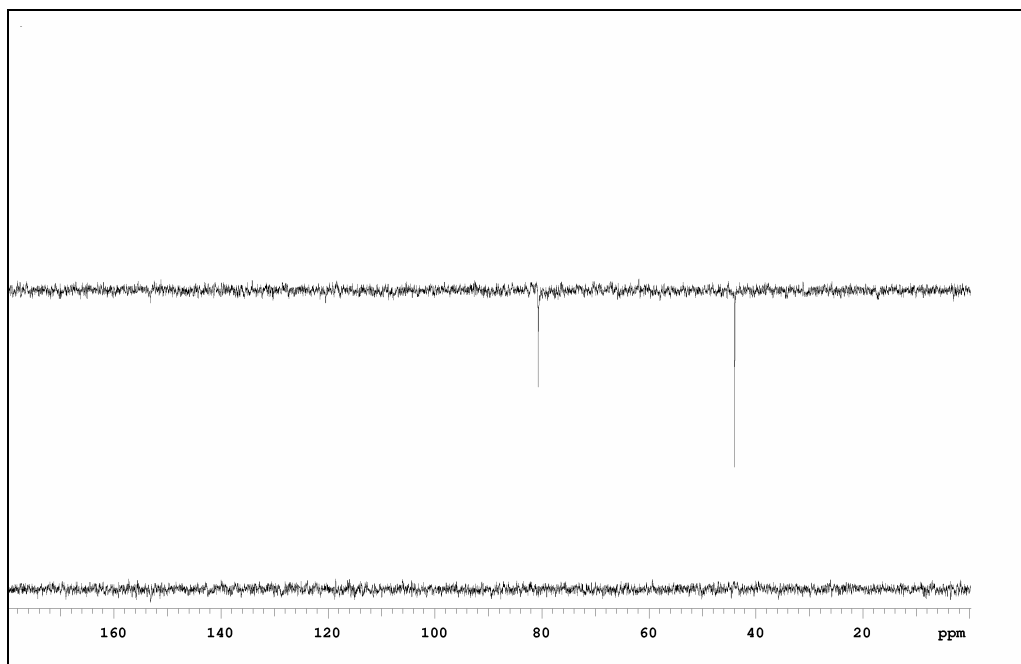
$^1\text{H-RMN}$ (300 MHz, CDCl_3)



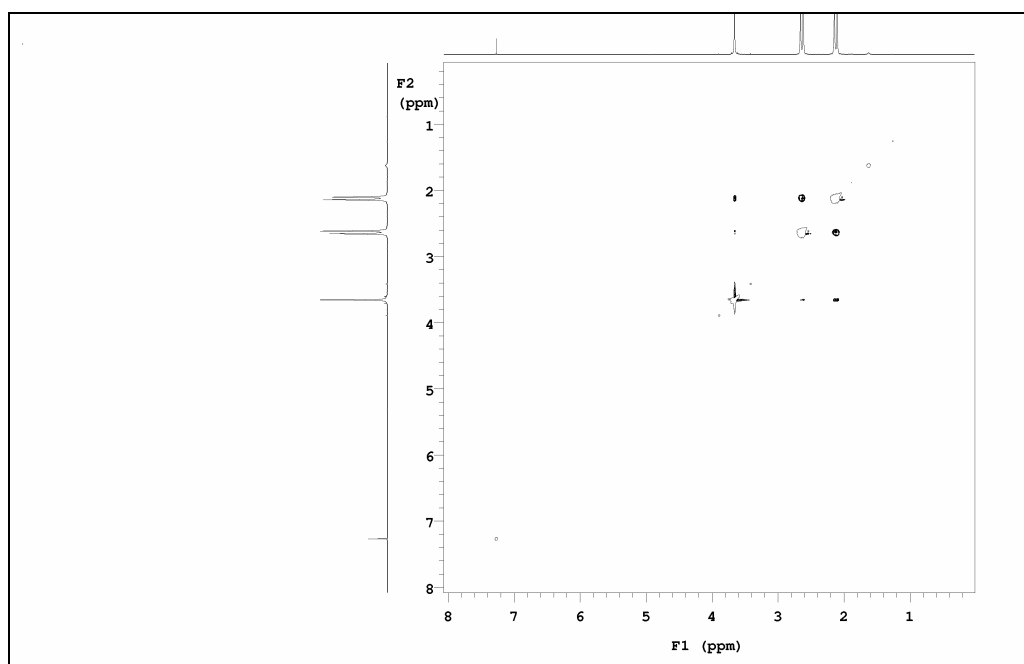
$^{13}\text{C-RMN}$ (75.4 MHz, CDCl_3)



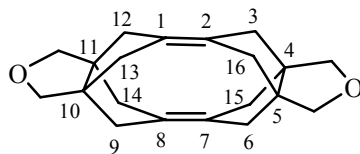
181



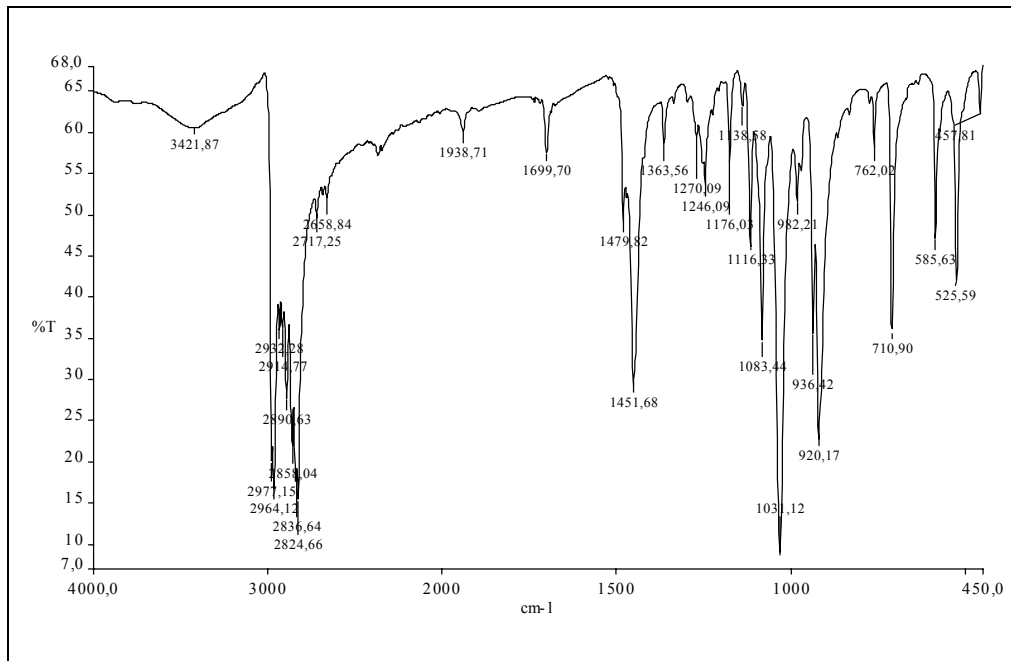
^{13}C -DEPT



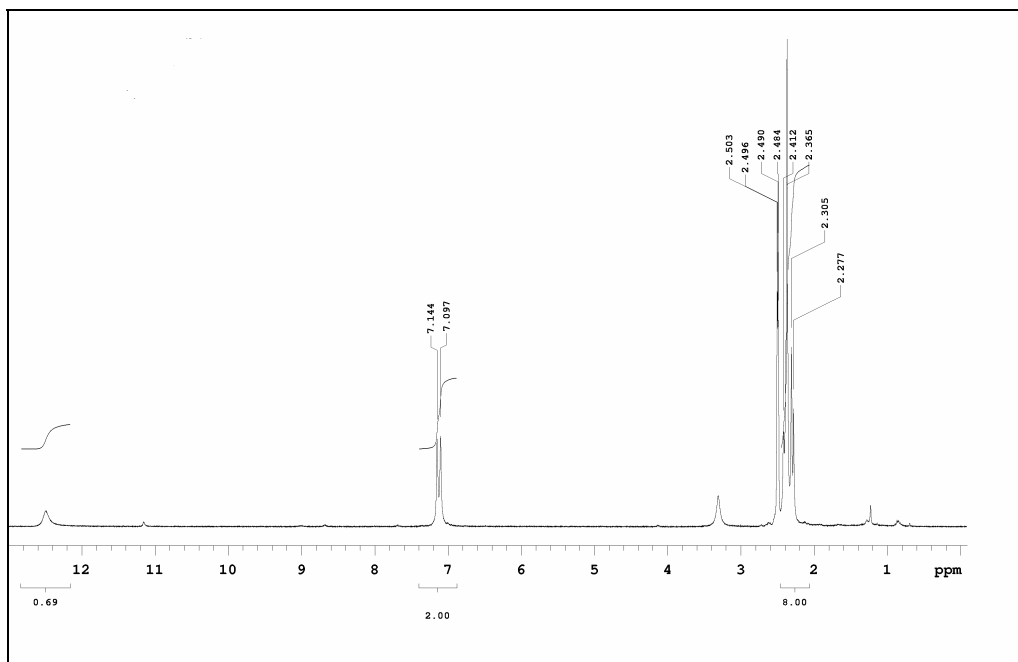
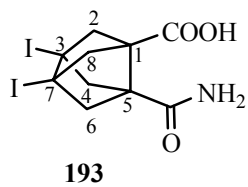
^1H - ^1H -NOESY



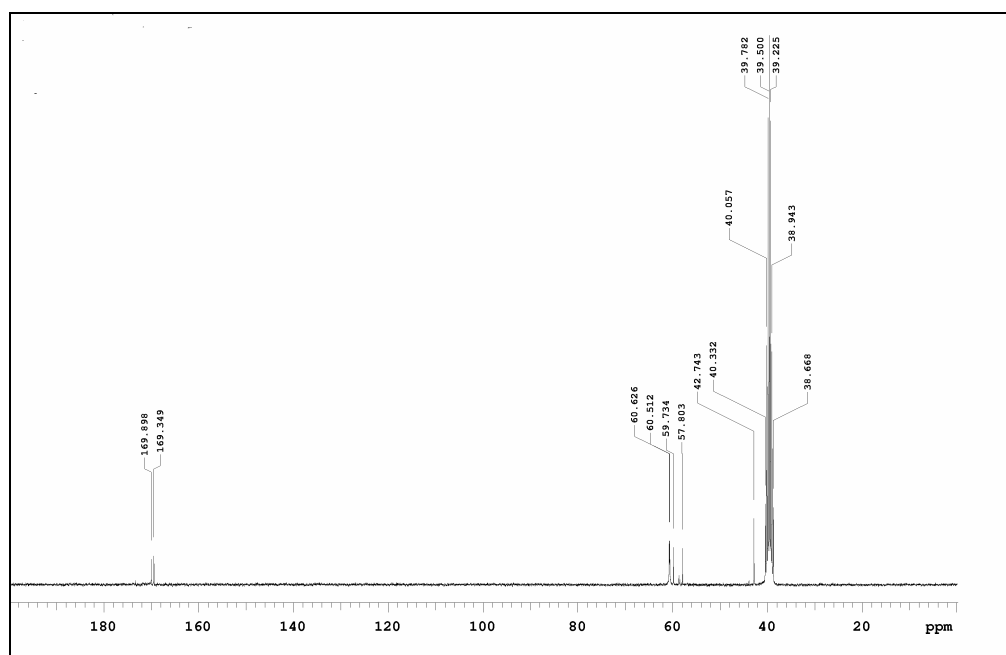
181



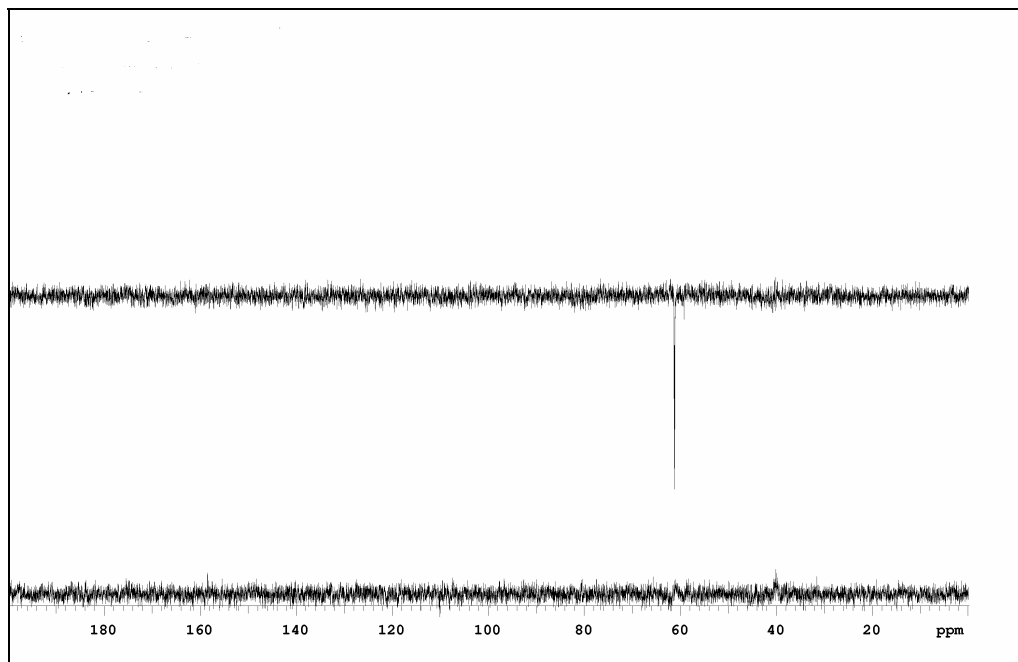
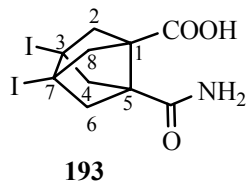
IR (KBr)



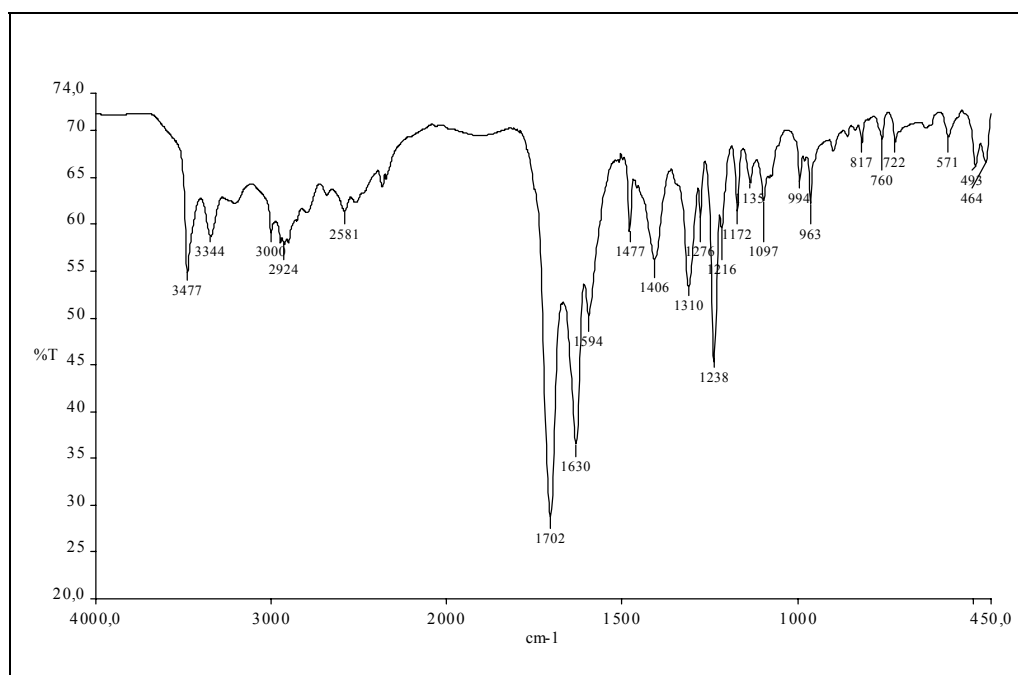
¹H-RMN (300 MHz, DMSO-d₆)



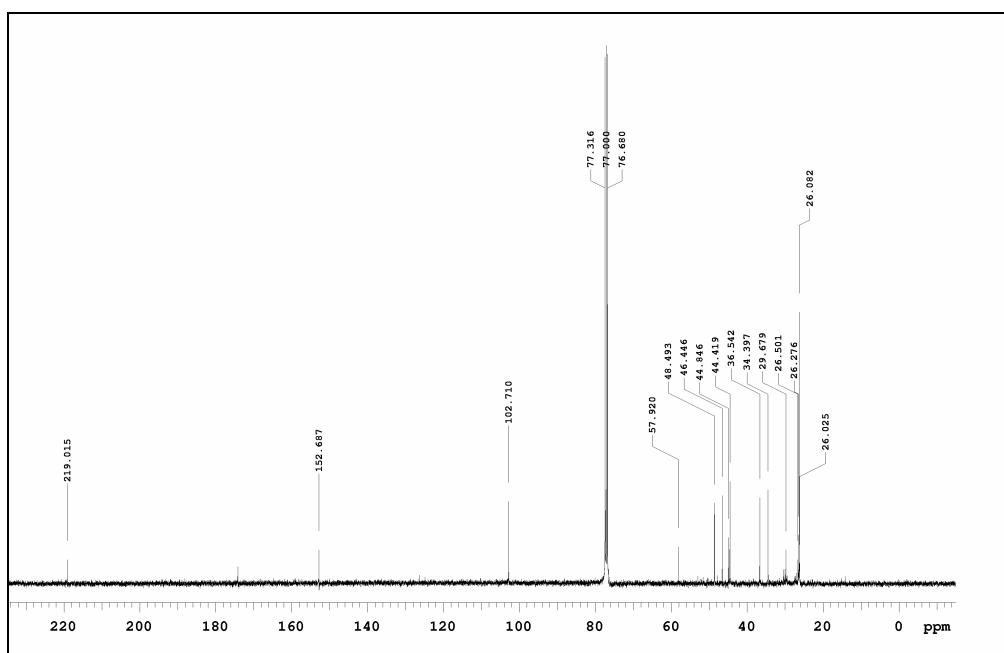
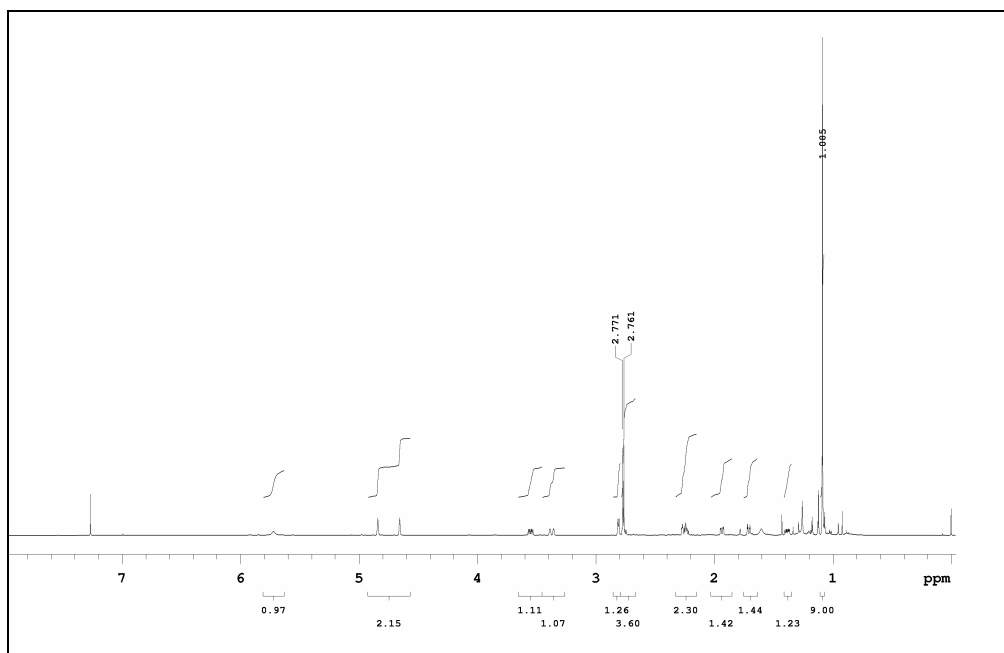
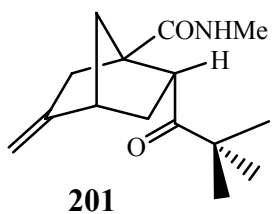
¹³C-RMN (75.4 MHz, DMSO-d₆)

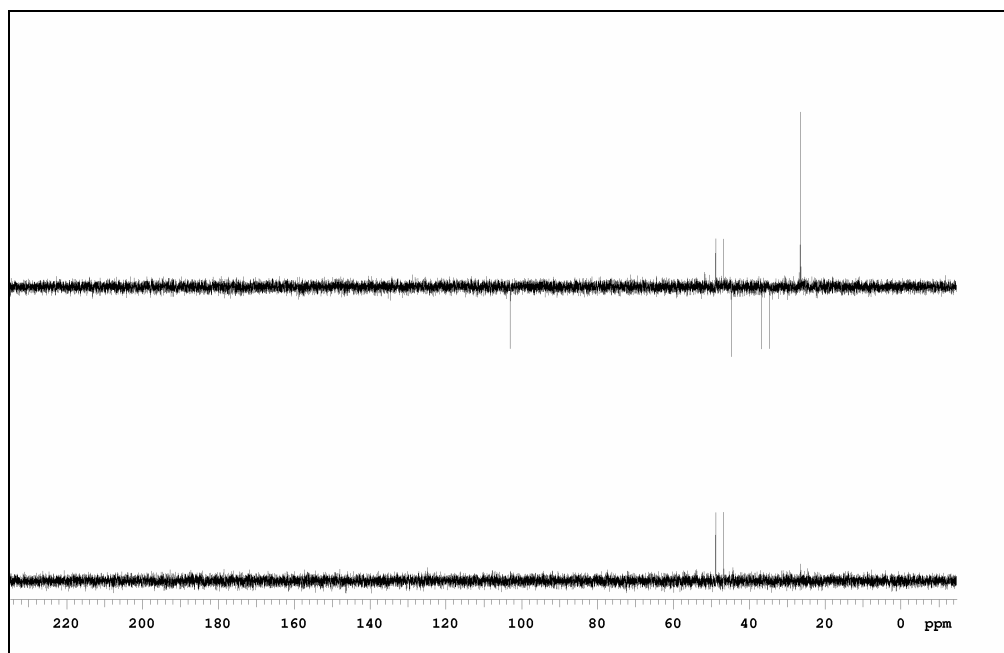
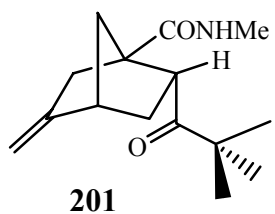


¹³C-DEPT

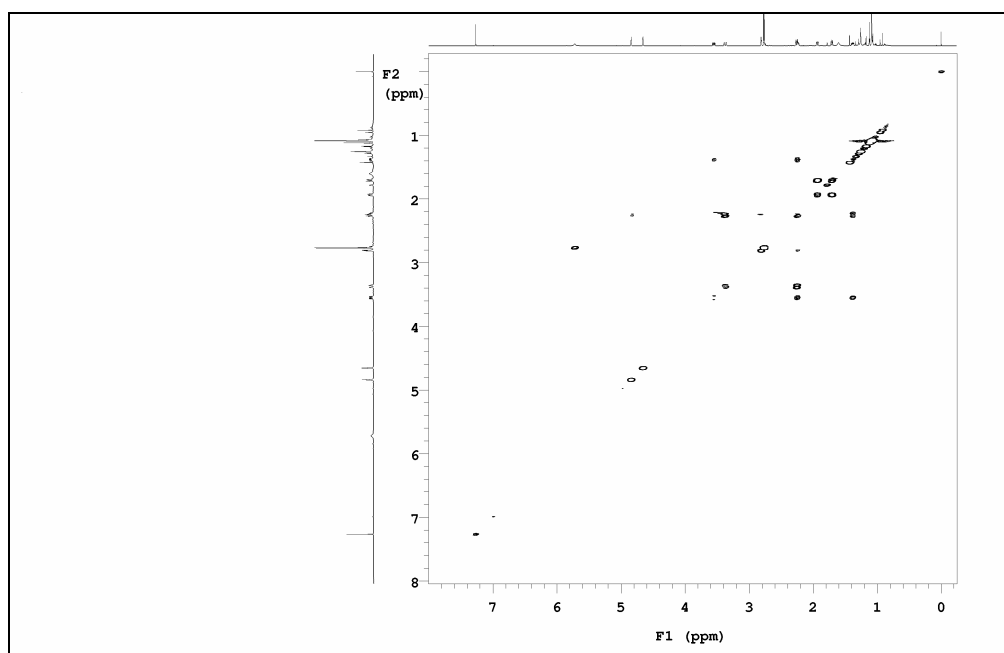


IR (KBr)

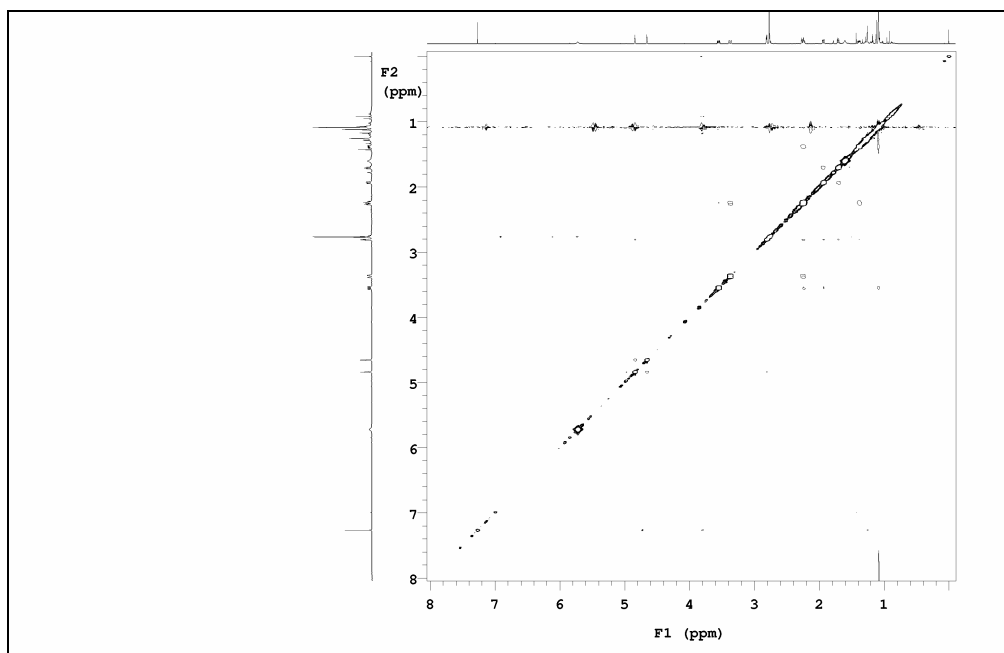
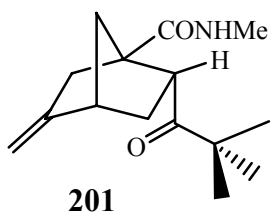
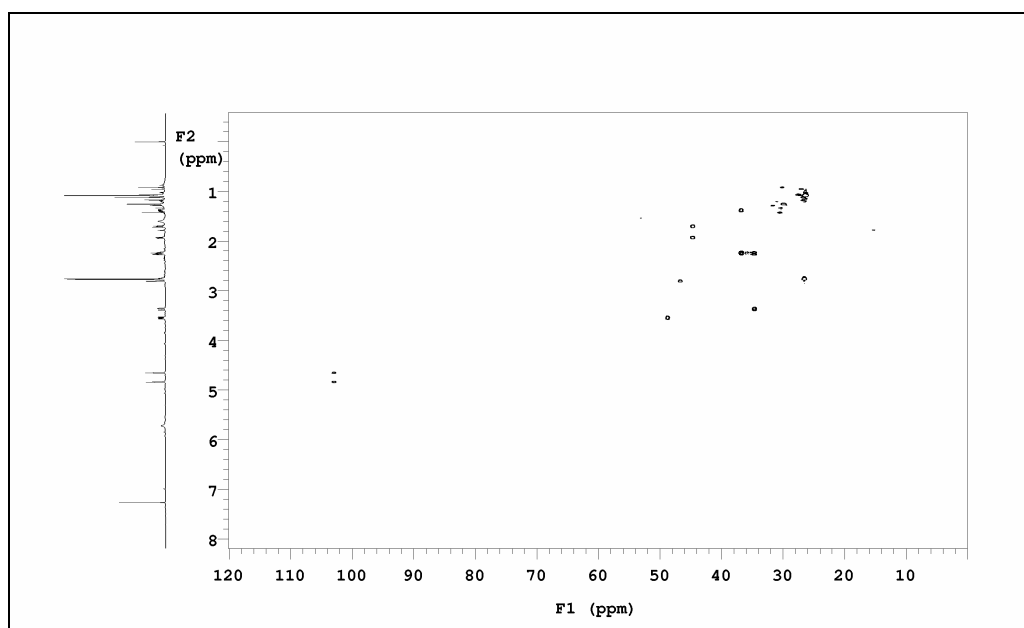


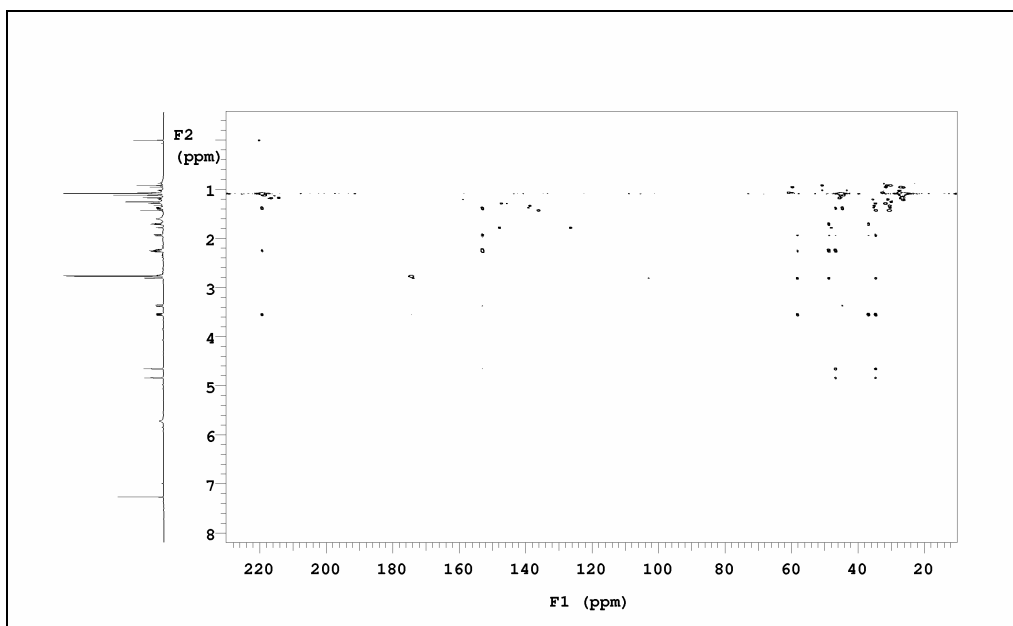
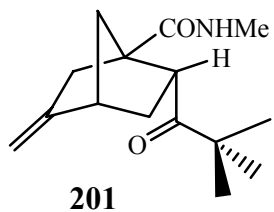


^{13}C -DEPT

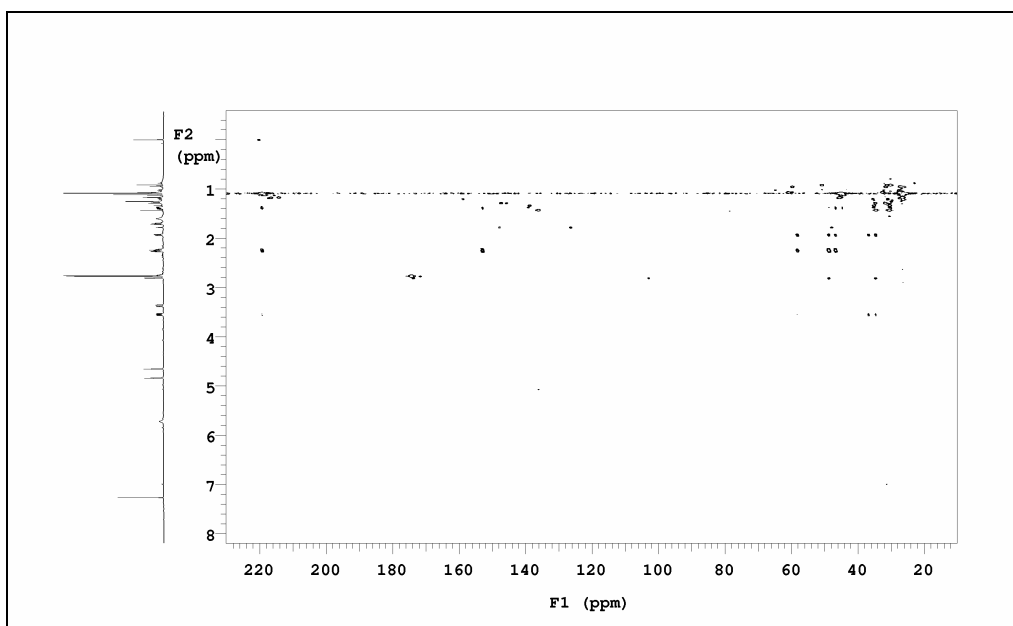


^1H - ^1H -COSY

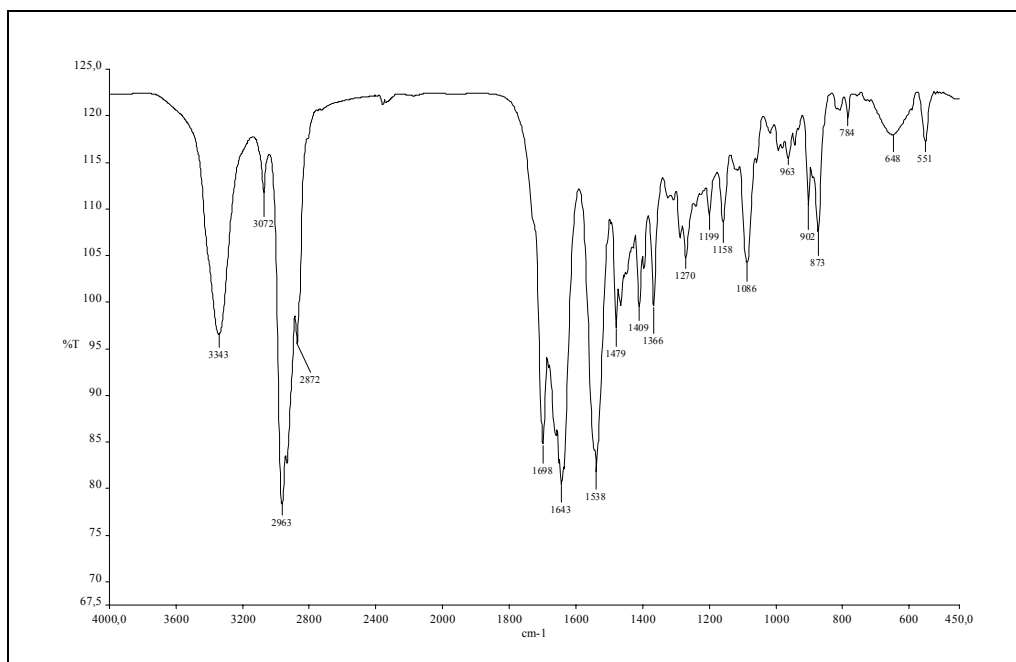
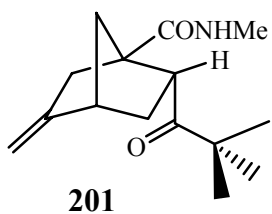
 ^1H - ^1H -NOESY ^1H - ^{13}C -HSQC



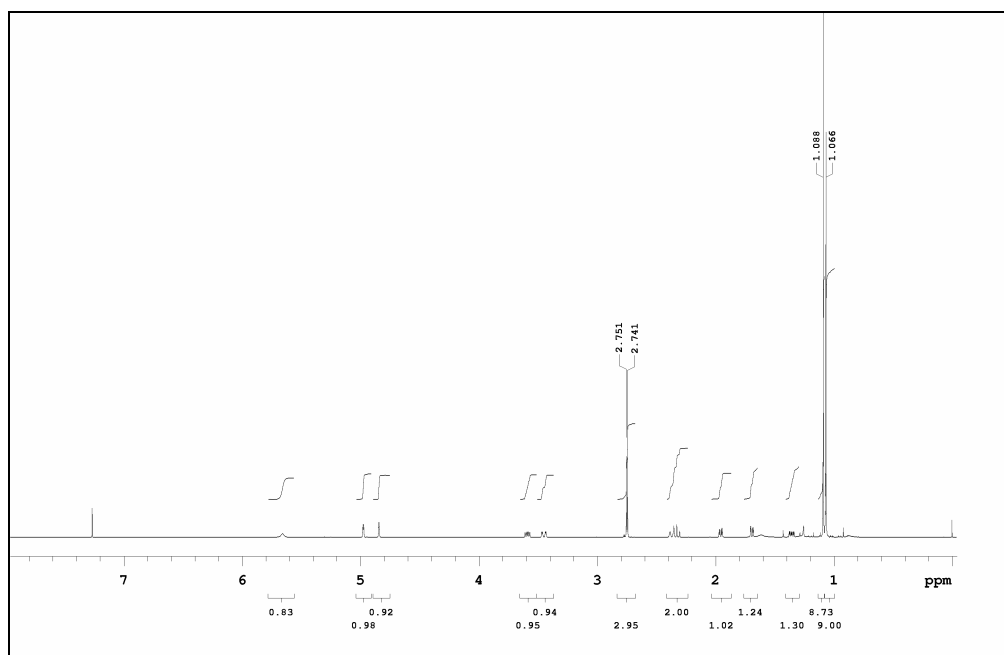
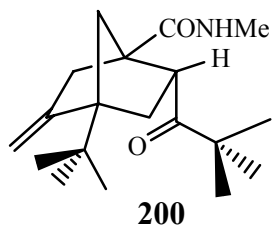
$^1\text{H}-^{13}\text{C}\text{-HMBC } J = 8 \text{ Hz}$



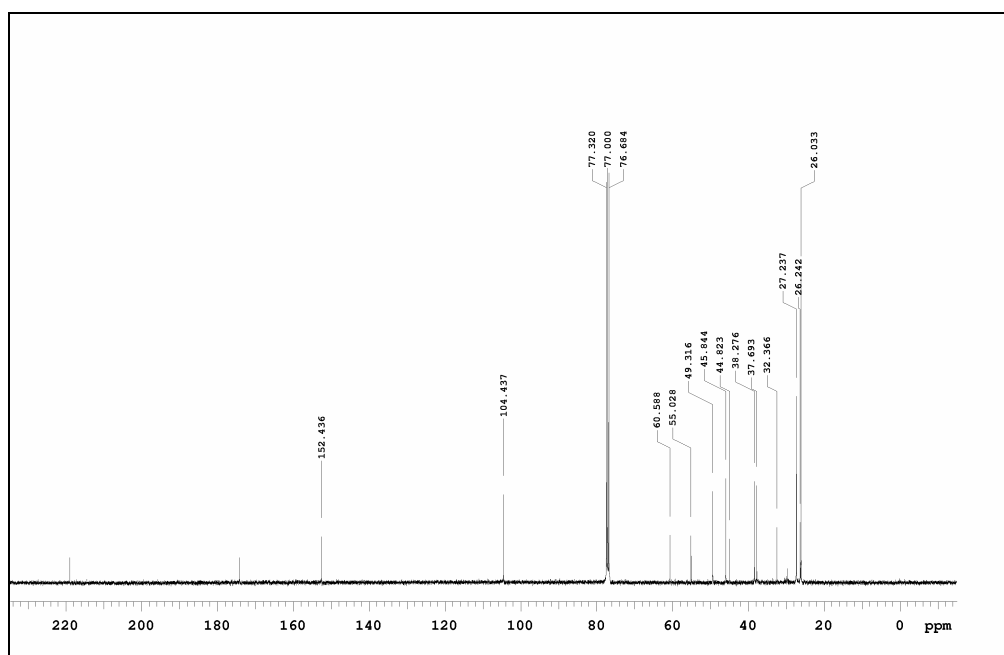
$^1\text{H}-^{13}\text{C}\text{-HMBC } J = 5 \text{ Hz}$



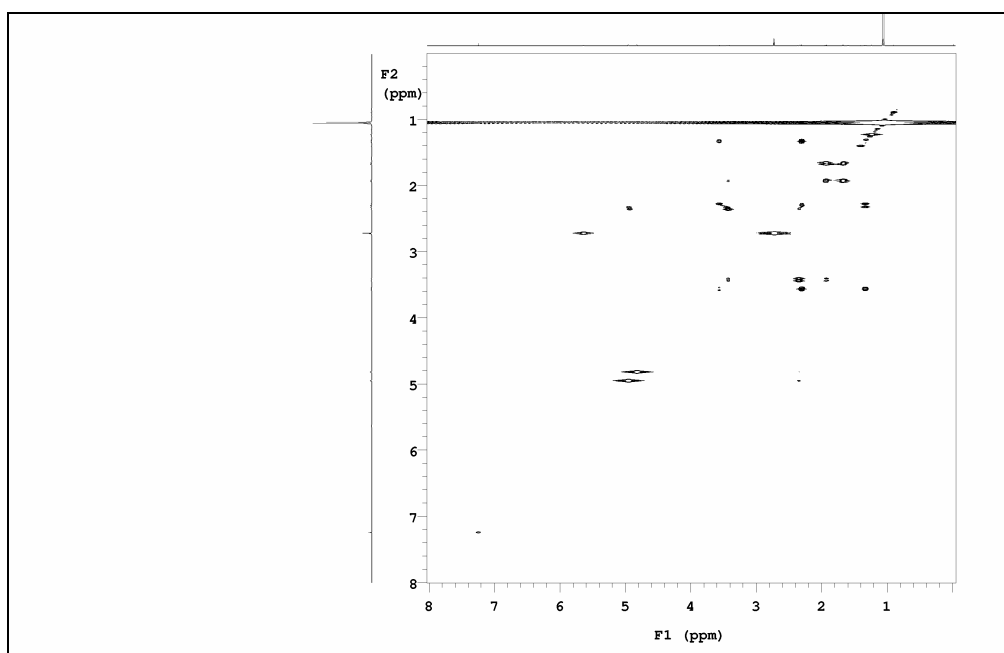
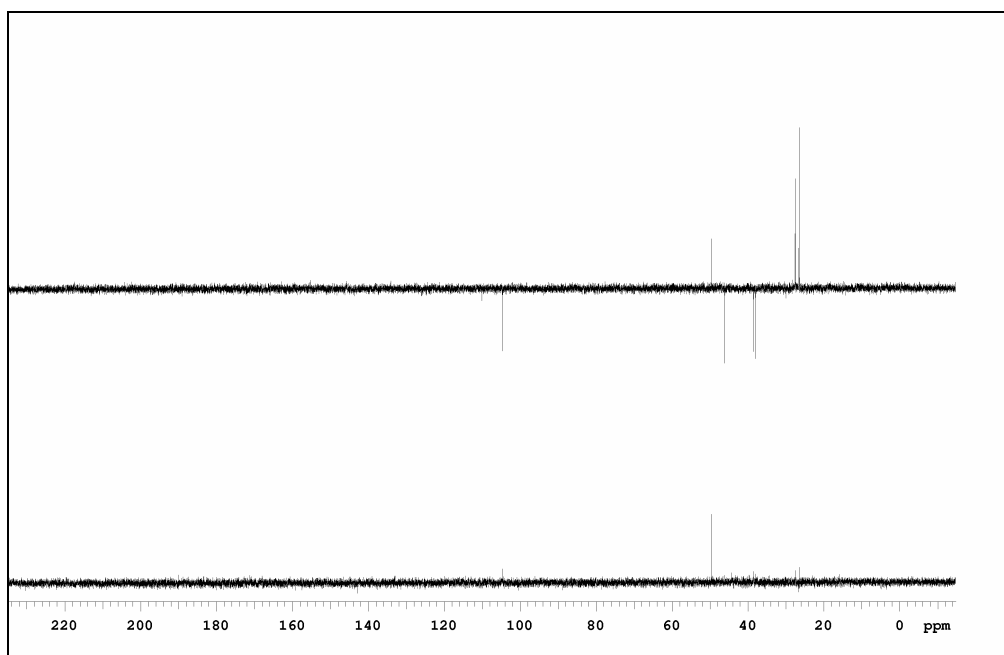
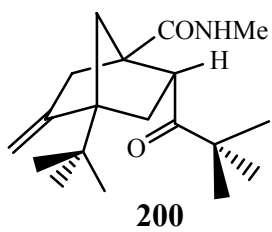
IR (NaCl)

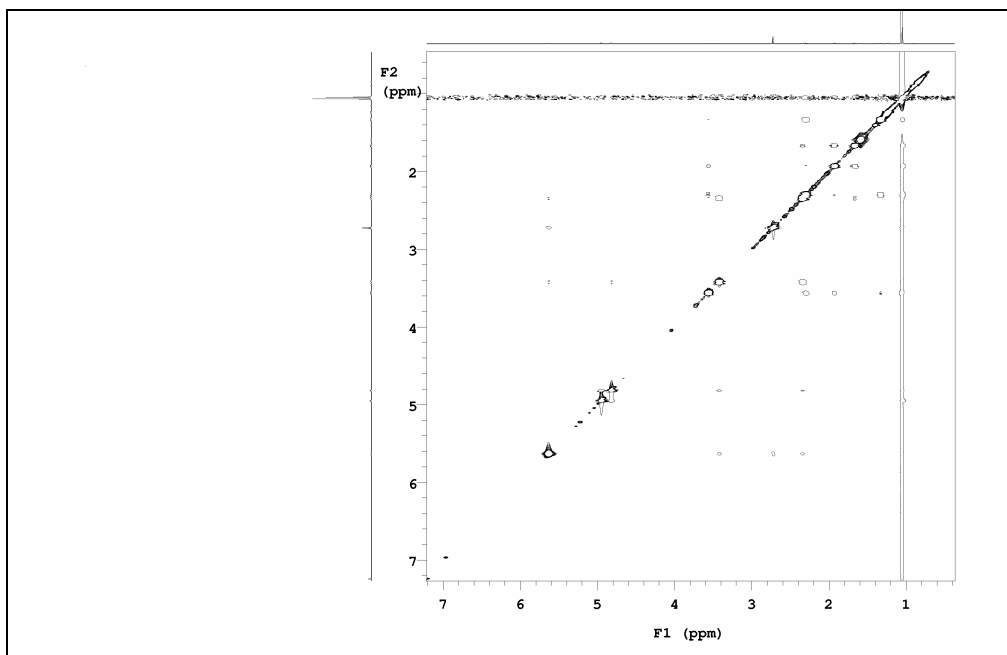
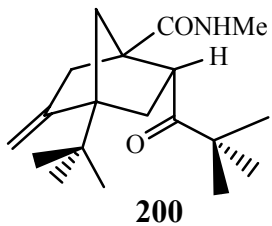


$^1\text{H-RMN}$ (500 MHz, CDCl_3)

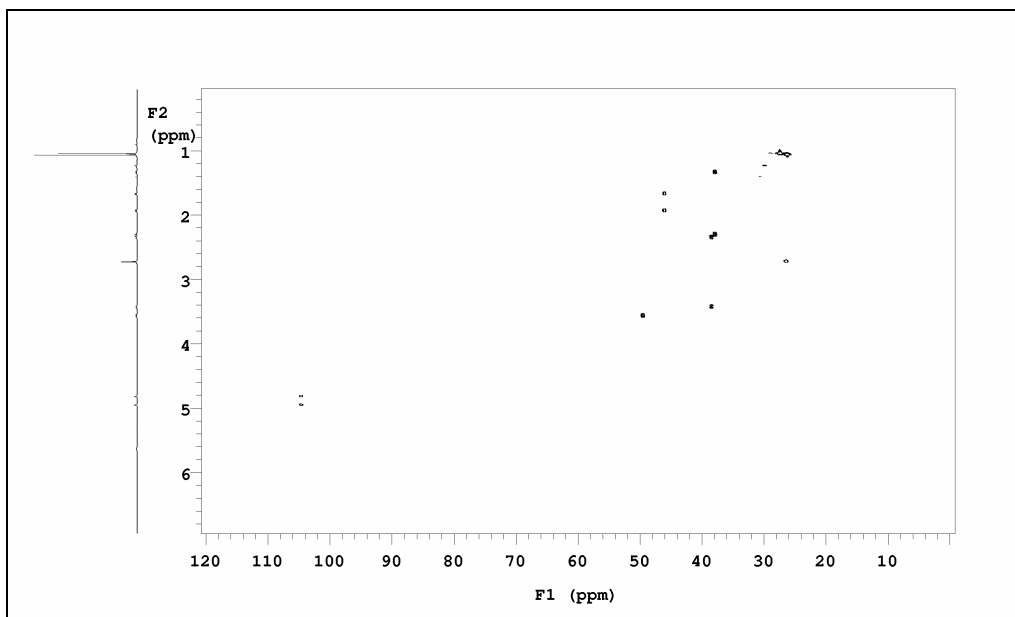


$^{13}\text{C-RMN}$ (100.6 MHz, CDCl_3)

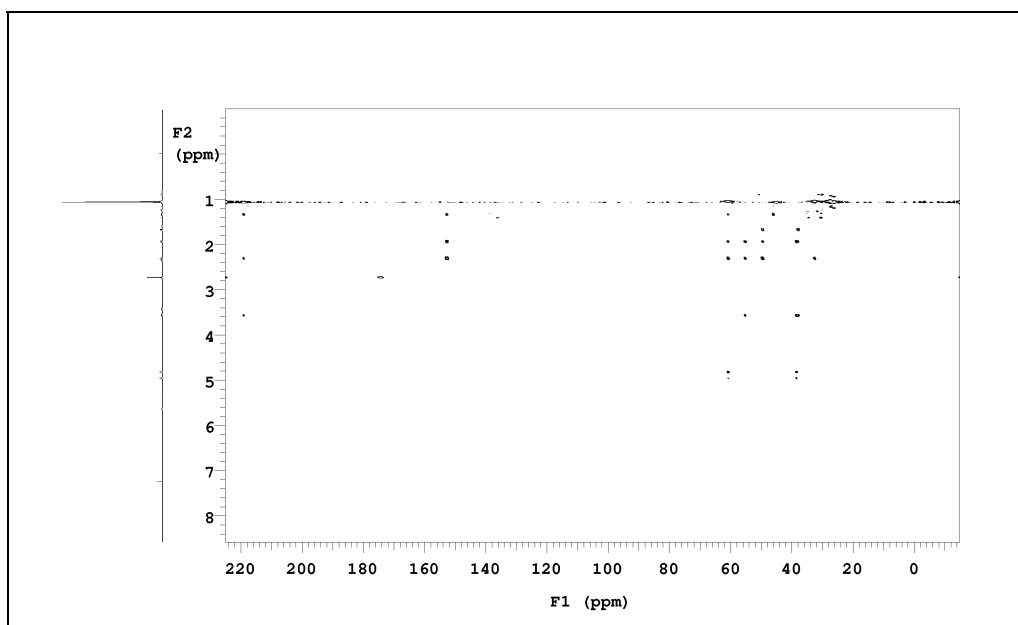
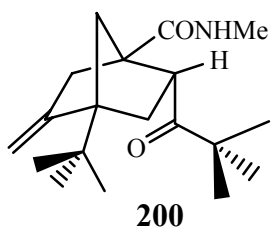




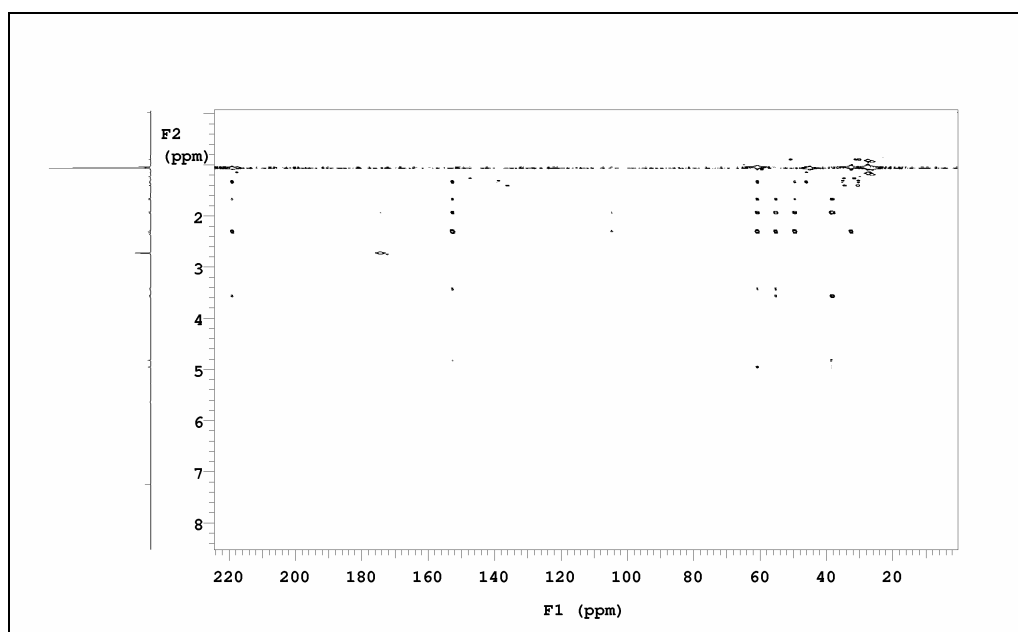
^1H - ^1H -NOESY



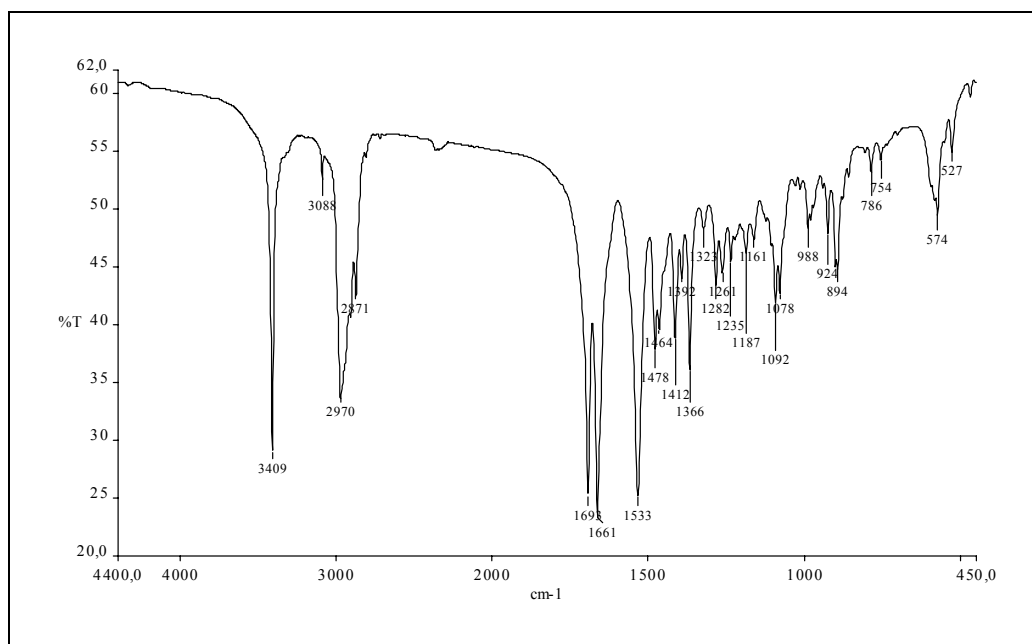
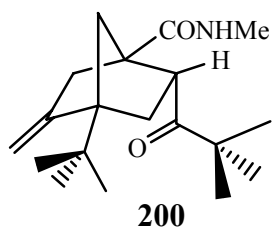
^1H - ^{13}C -HSQC



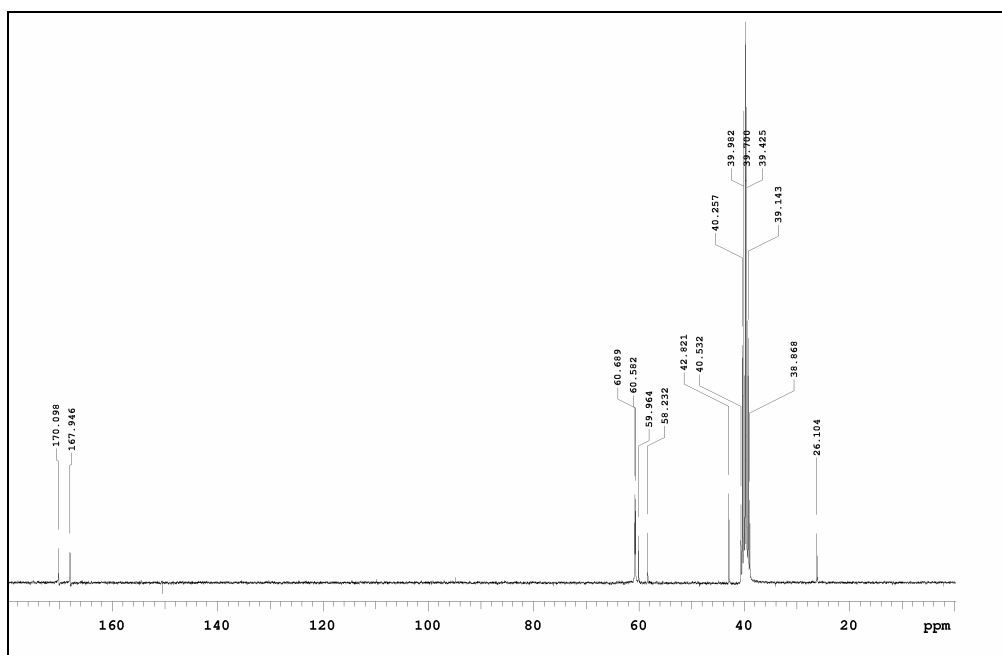
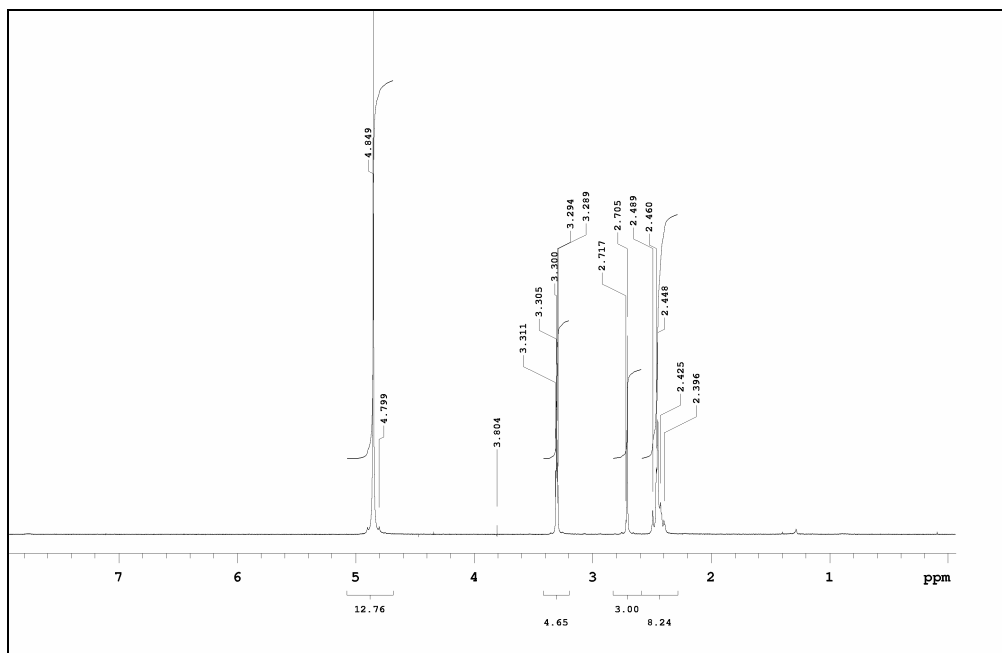
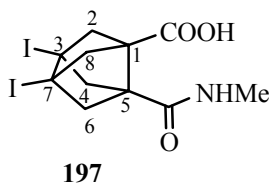
$^1\text{H}-^{13}\text{C}$ -HMBC $J = 8 \text{ Hz}$

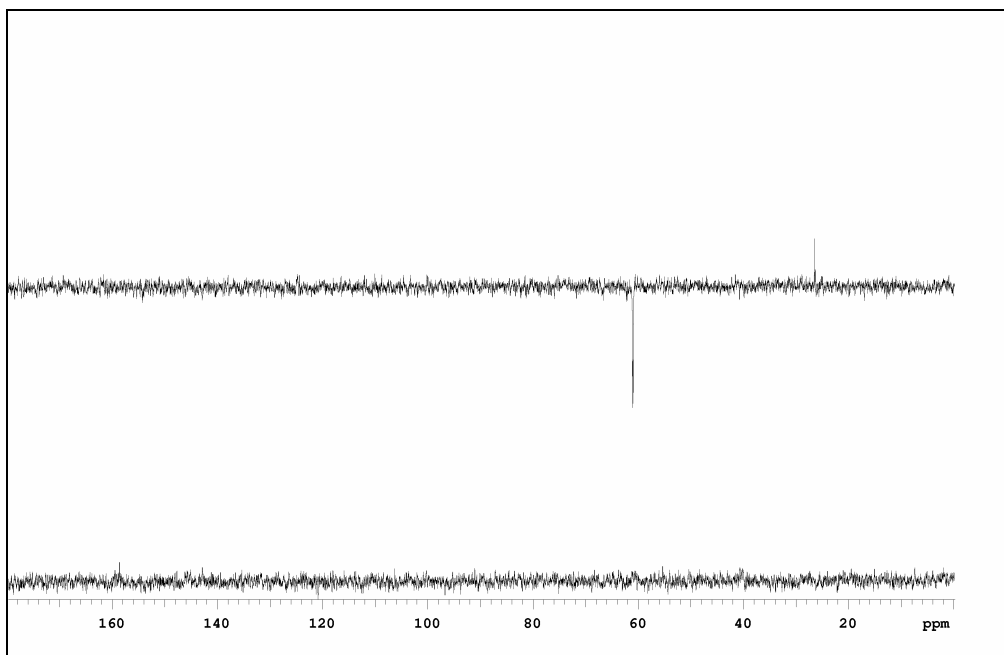
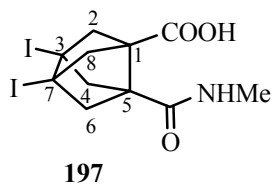


$^1\text{H}-^{13}\text{C}$ -HMBC $J = 5 \text{ Hz}$

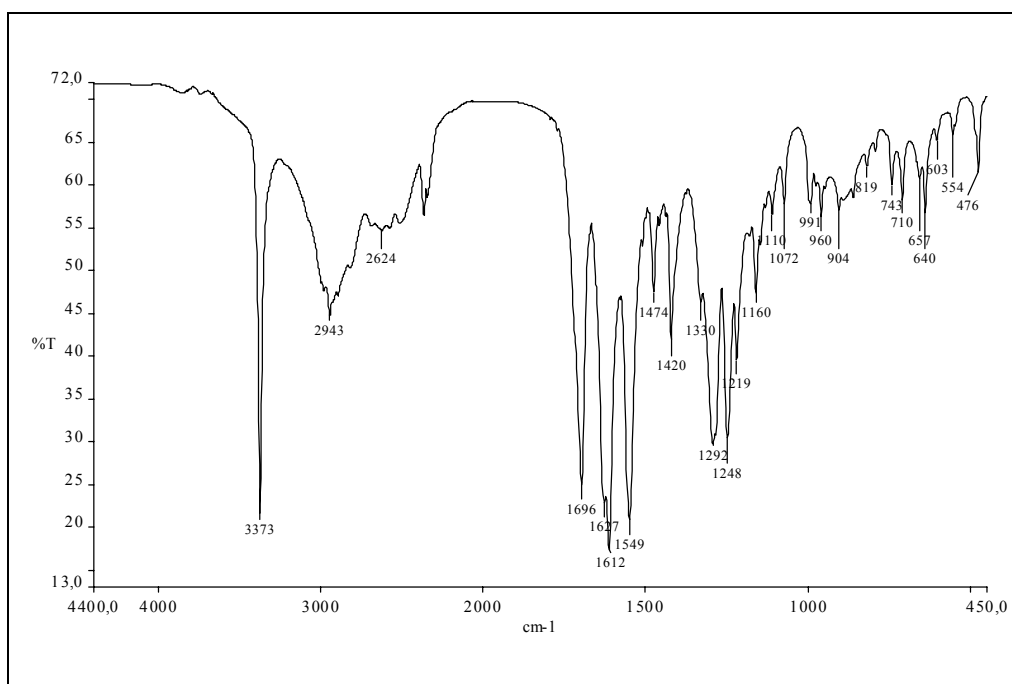


IR (KBr)

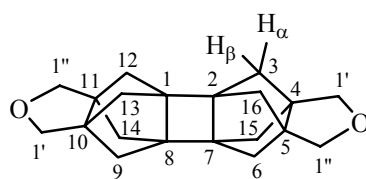




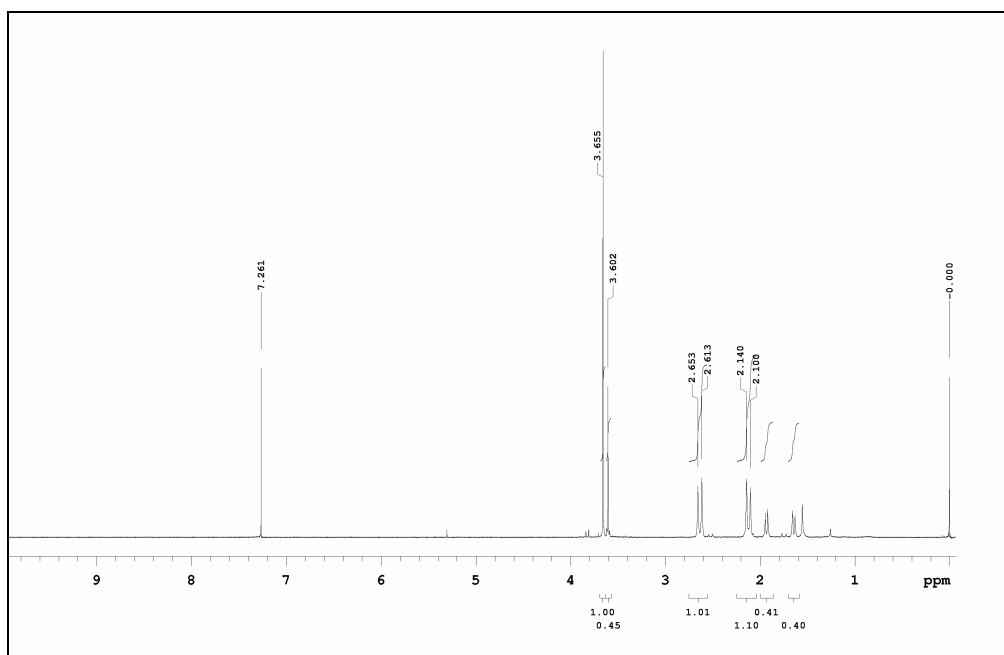
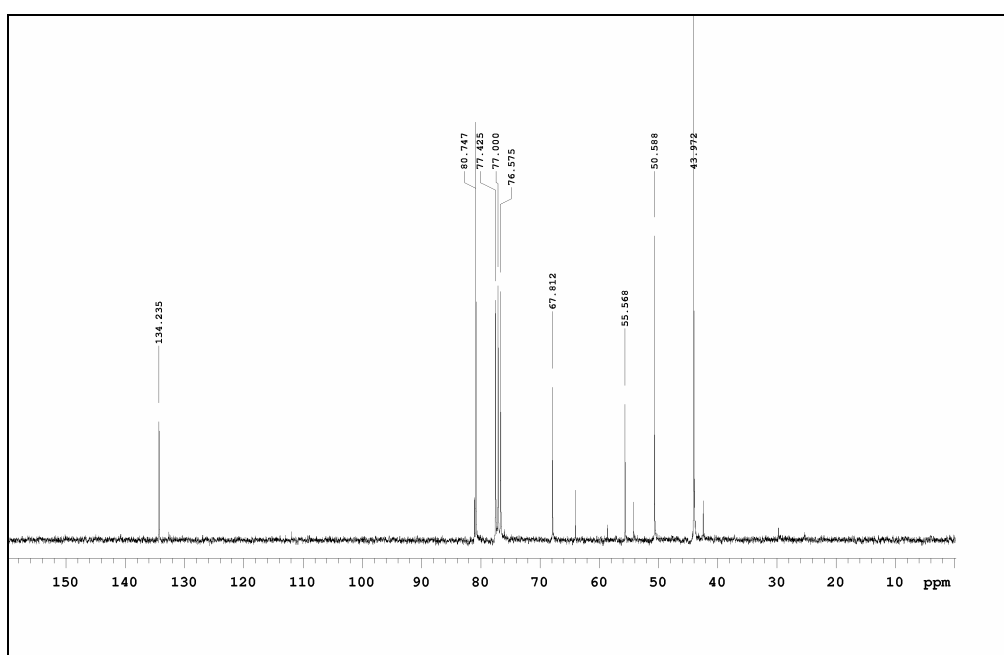
¹³C-DEPT

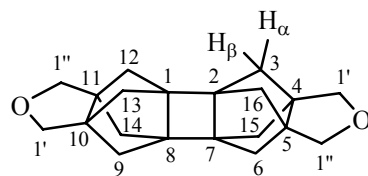


IR (KBr)

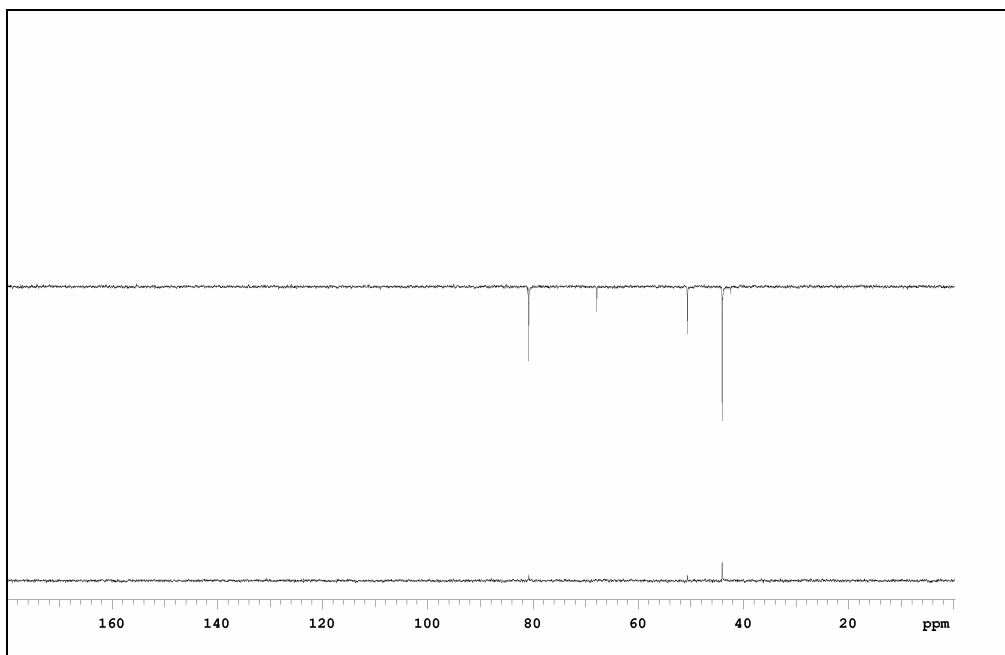


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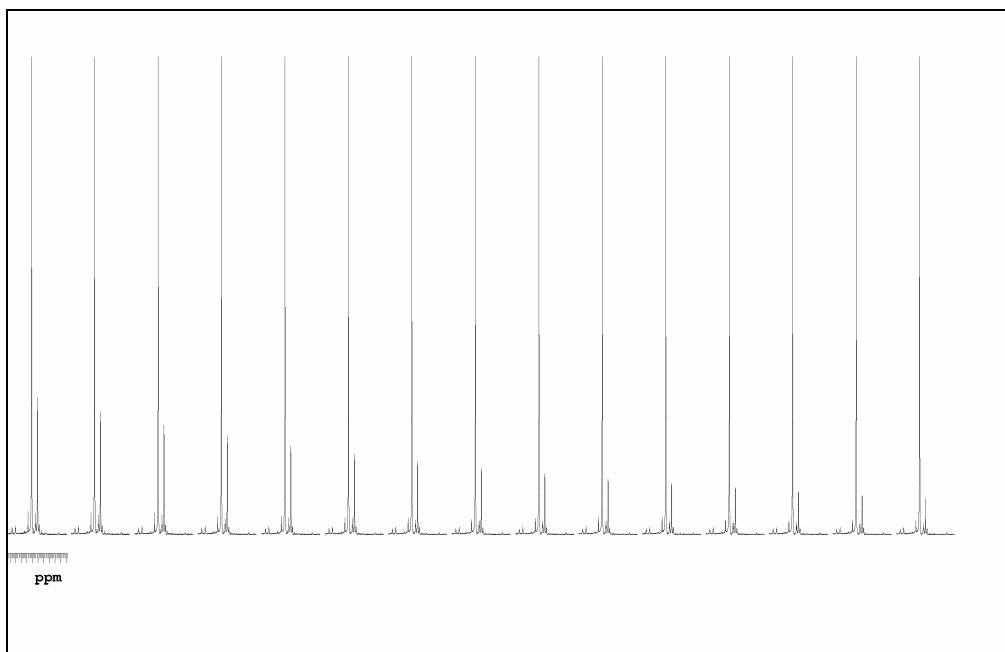
¹H-RMN (300 MHz, CDCl₃)¹³C-RMN (75.4 MHz, CDCl₃)



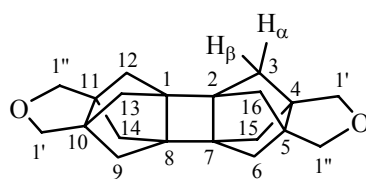
137



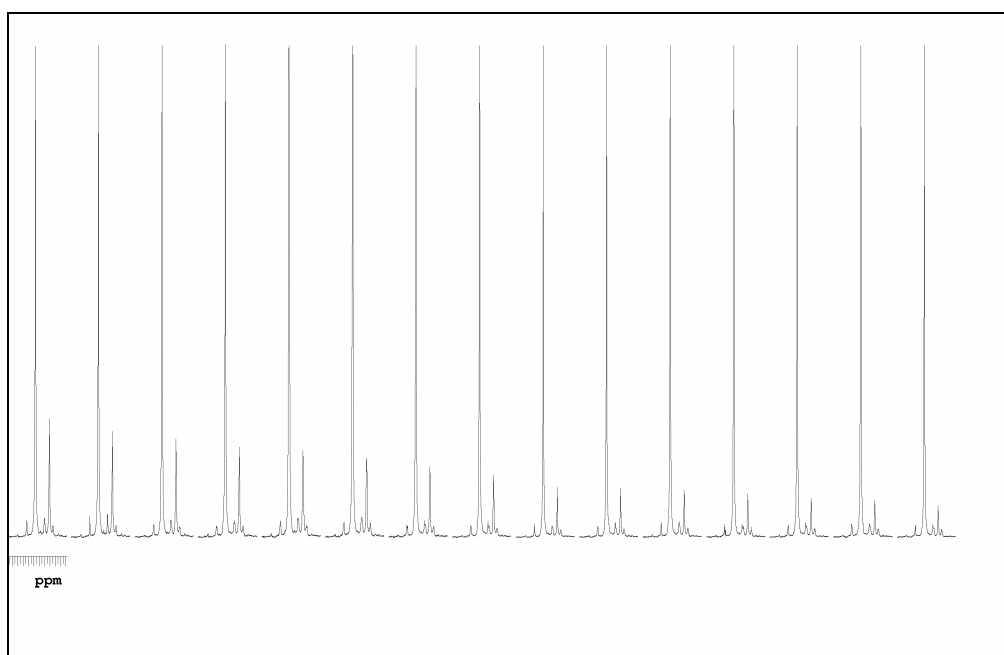
^{13}C -DEPT

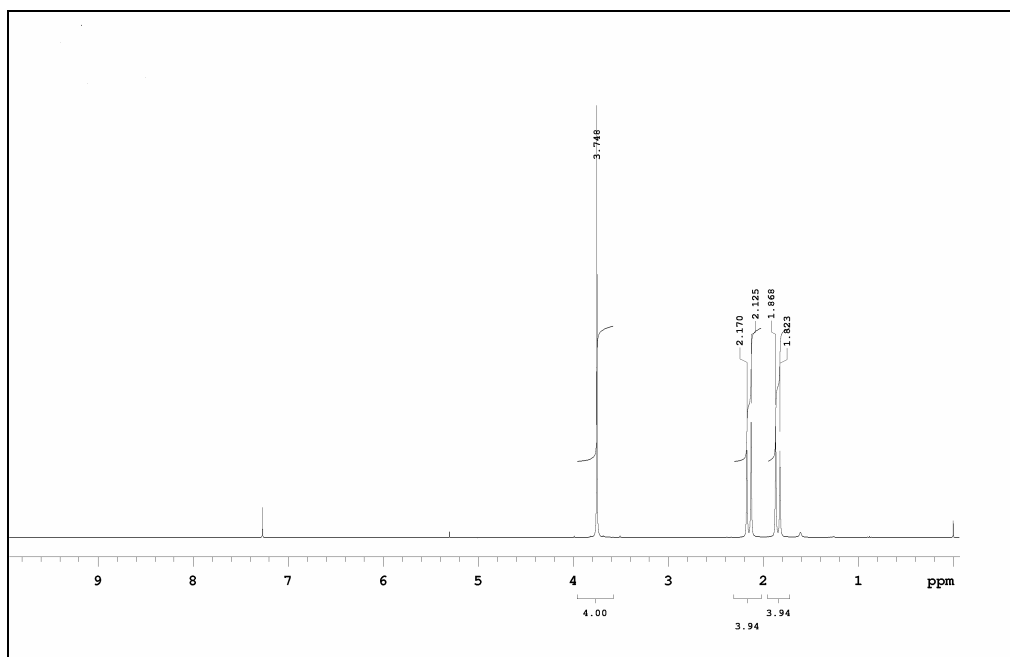
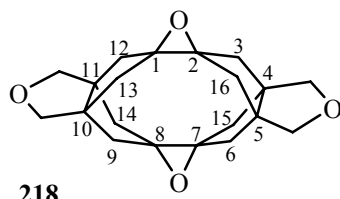


cinética de ^1H a 45°C

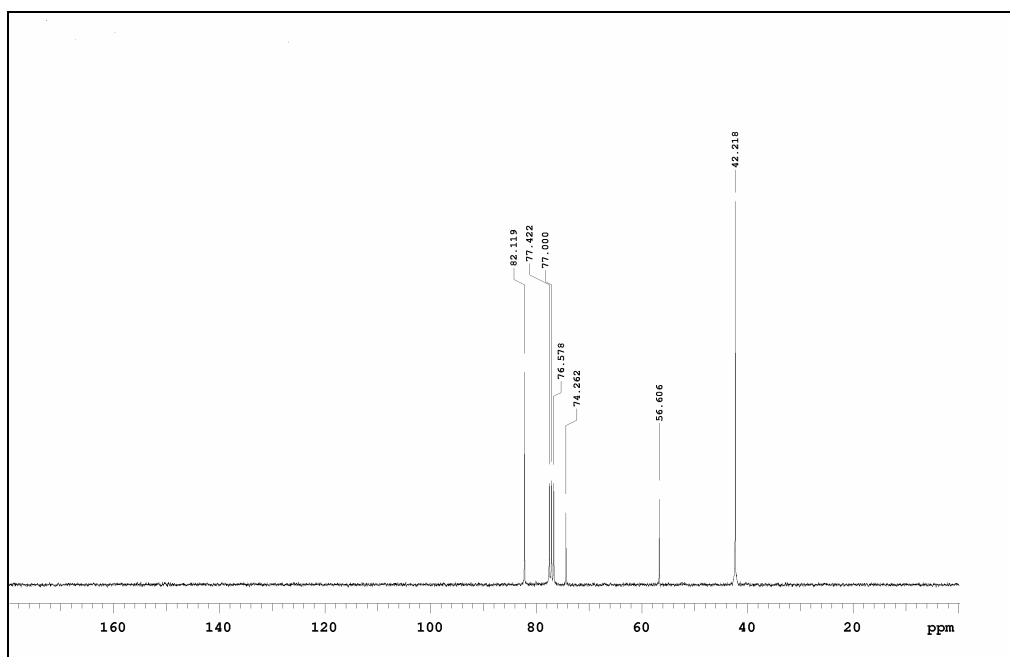


137

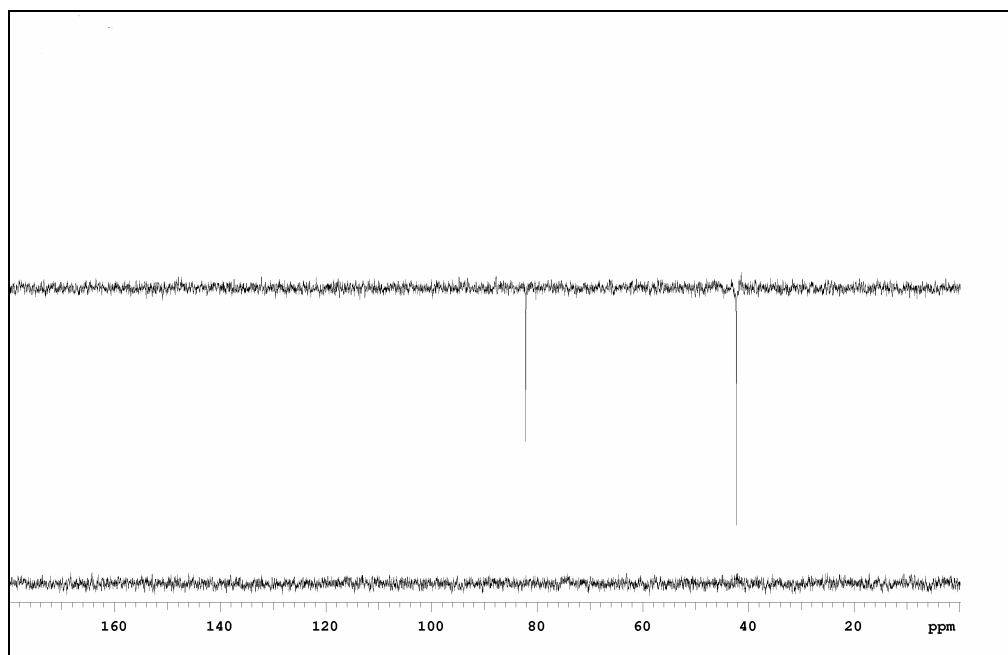
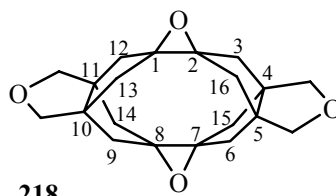
cinética de ¹H a 50°C



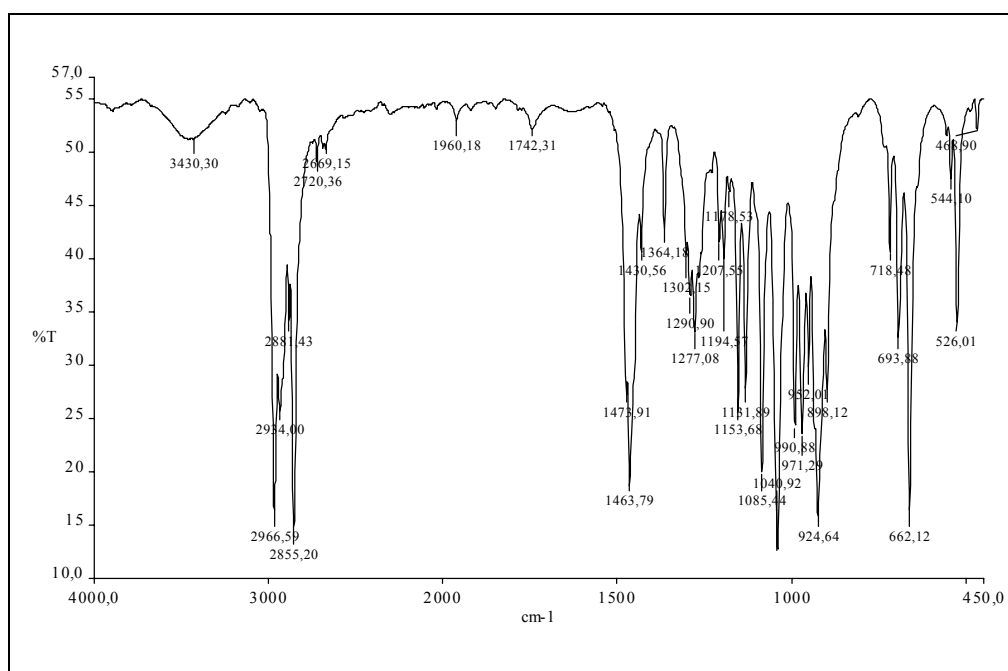
$^1\text{H-RMN}$ (300 MHz, CDCl_3)



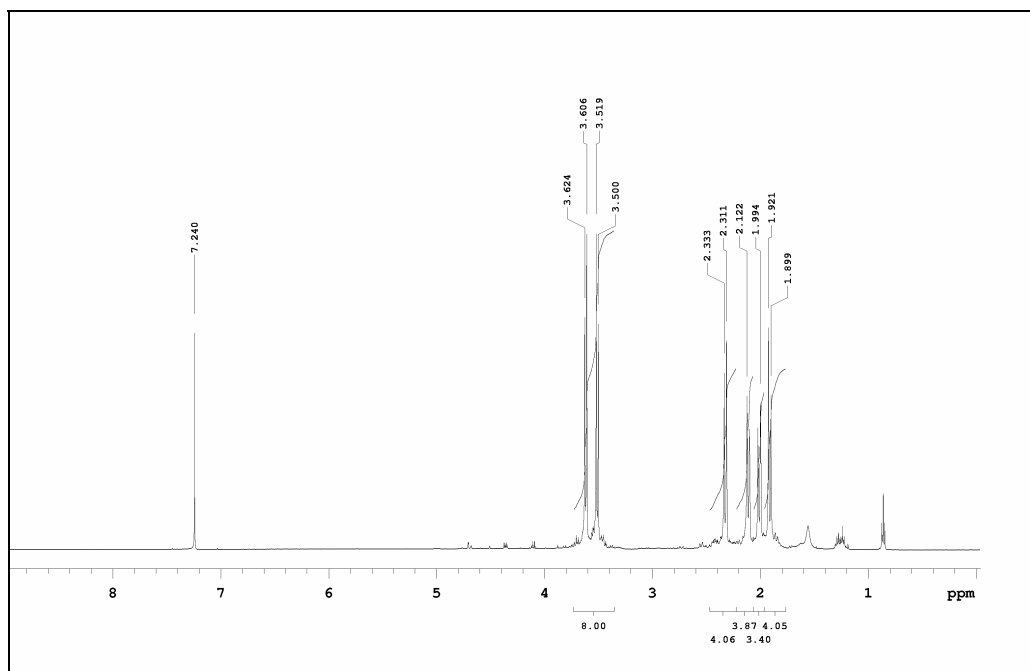
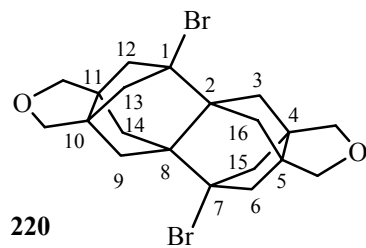
$^{13}\text{C-RMN}$ (75.4 MHz, CDCl_3)



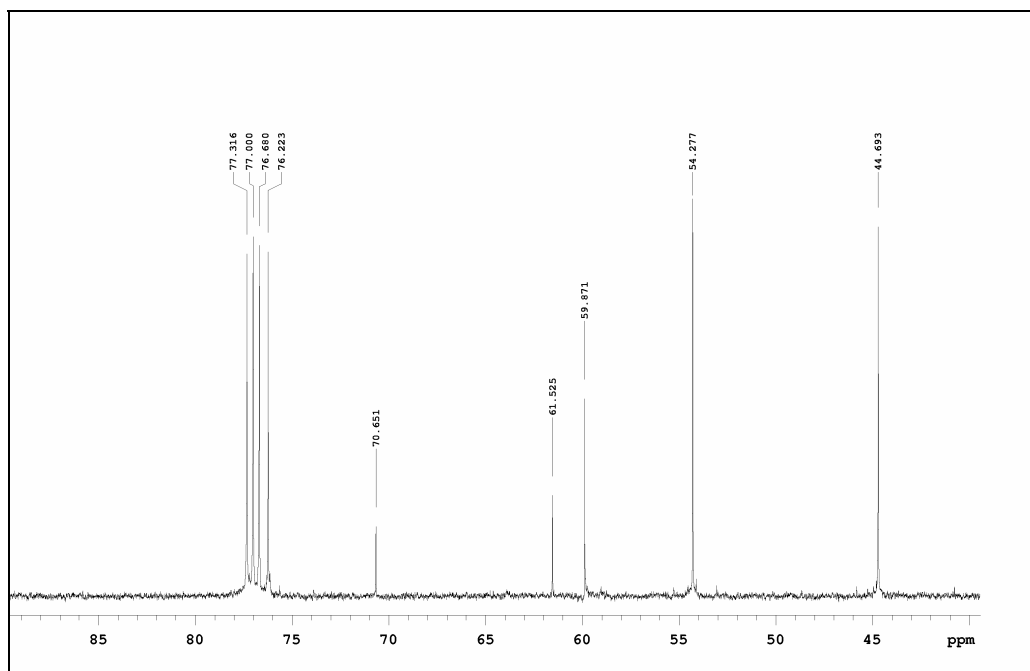
¹³C-DEPT



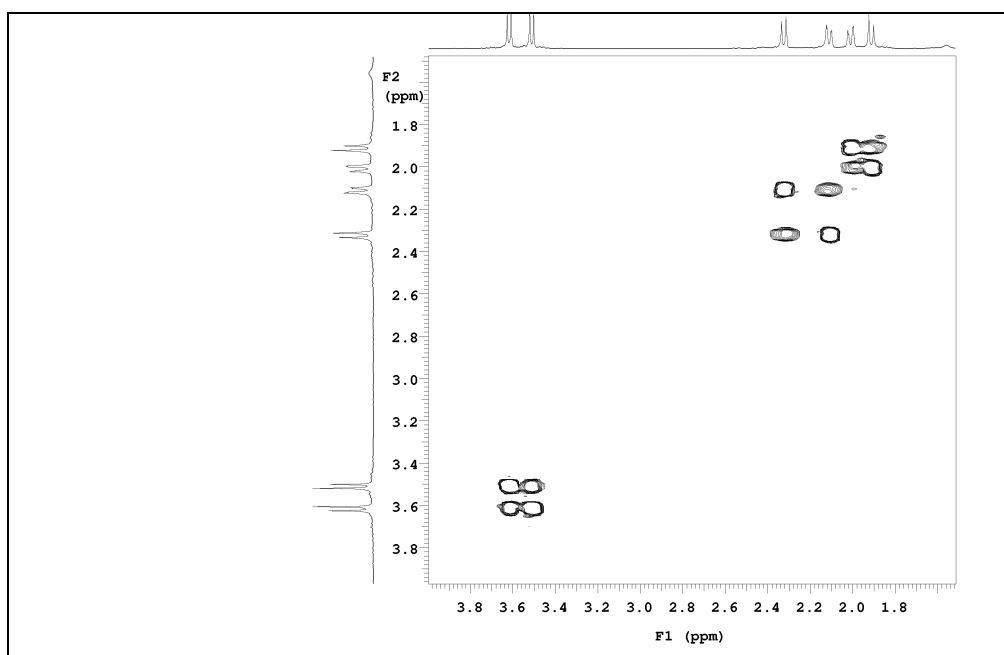
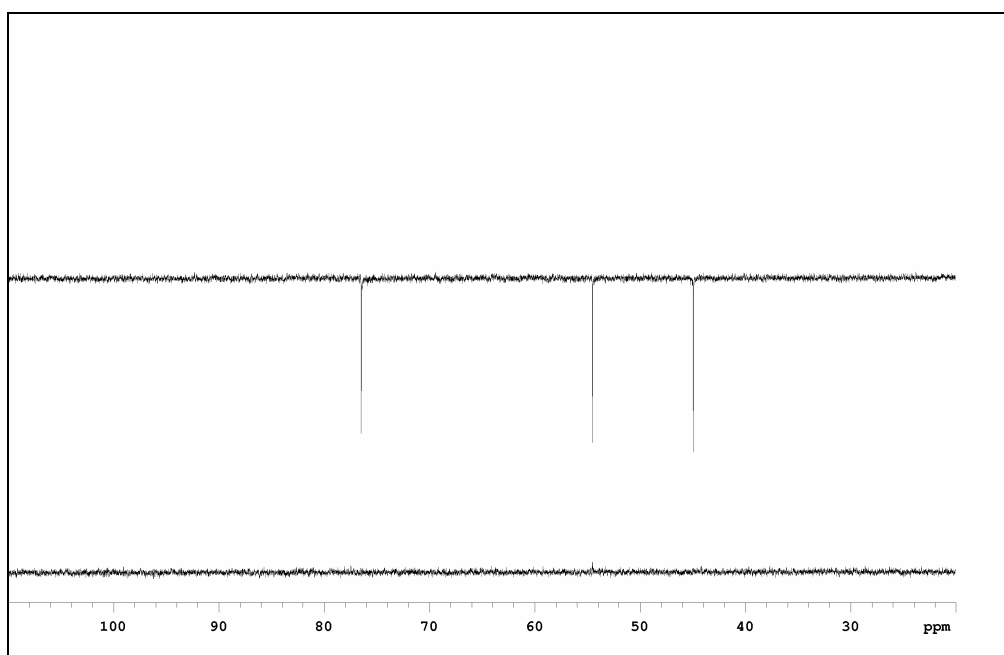
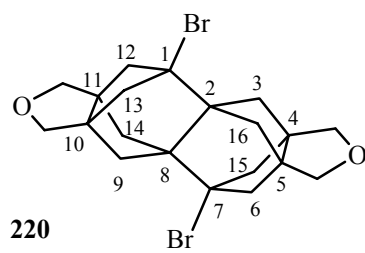
IR (KBr)

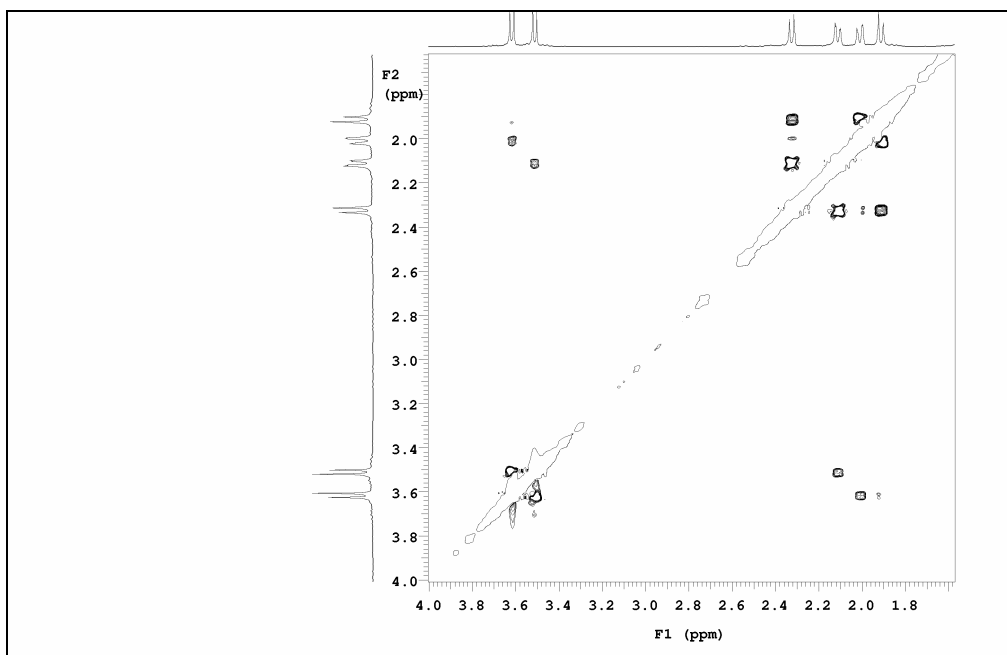
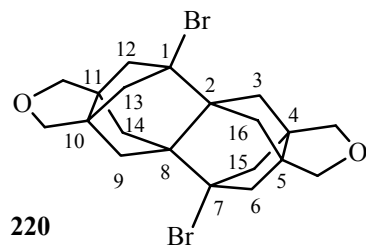


$^1\text{H-RMN}$ (500 MHz, CDCl_3)

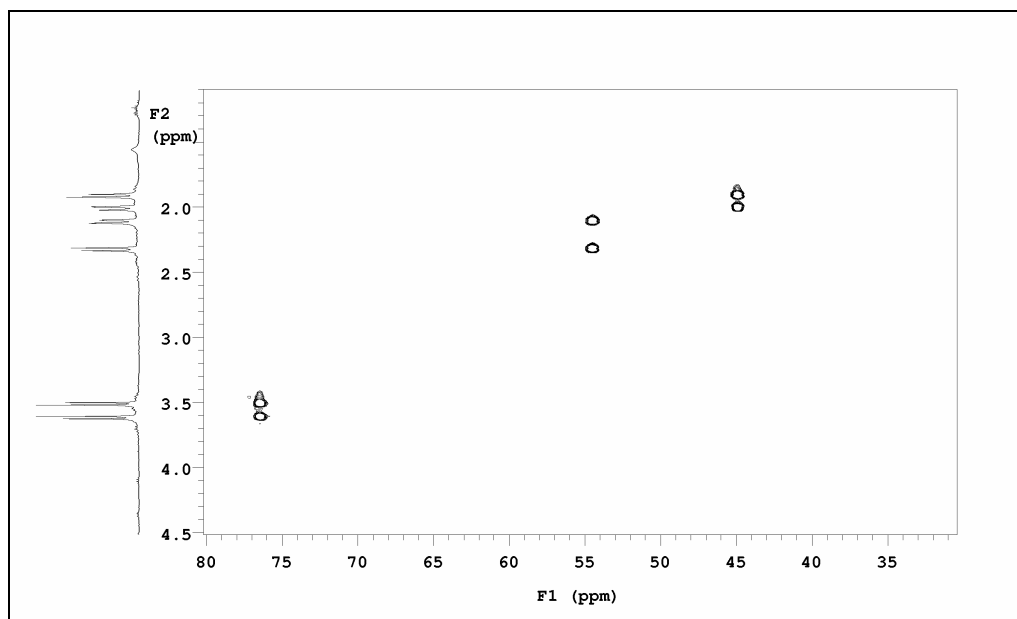


$^{13}\text{C-RMN}$ (100.6 MHz, CDCl_3)

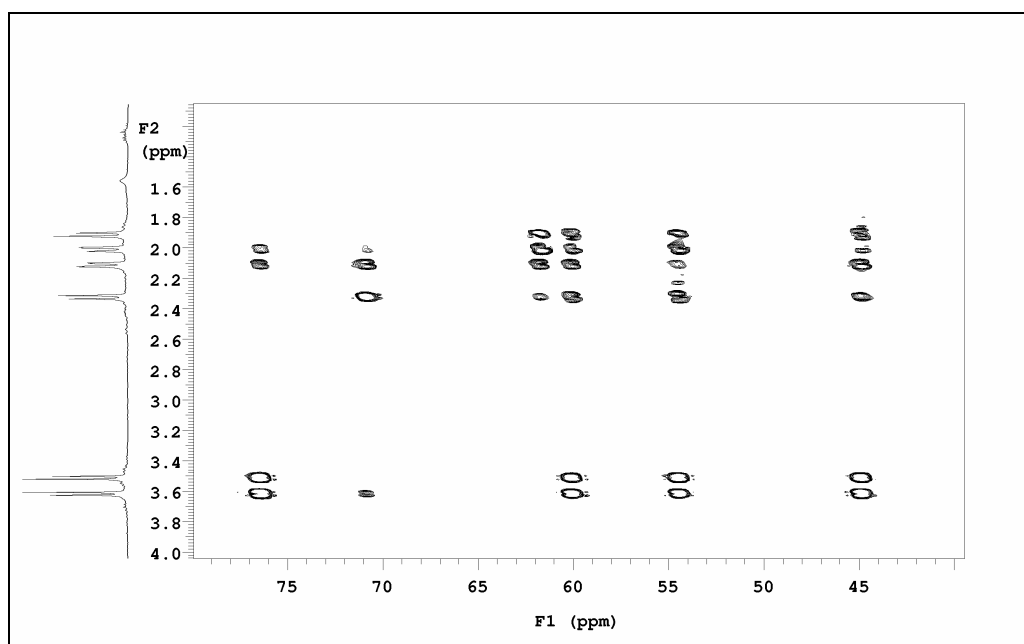
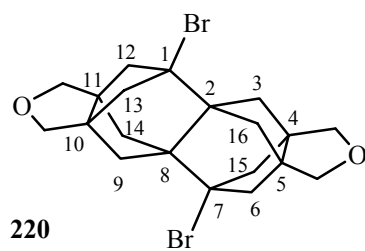




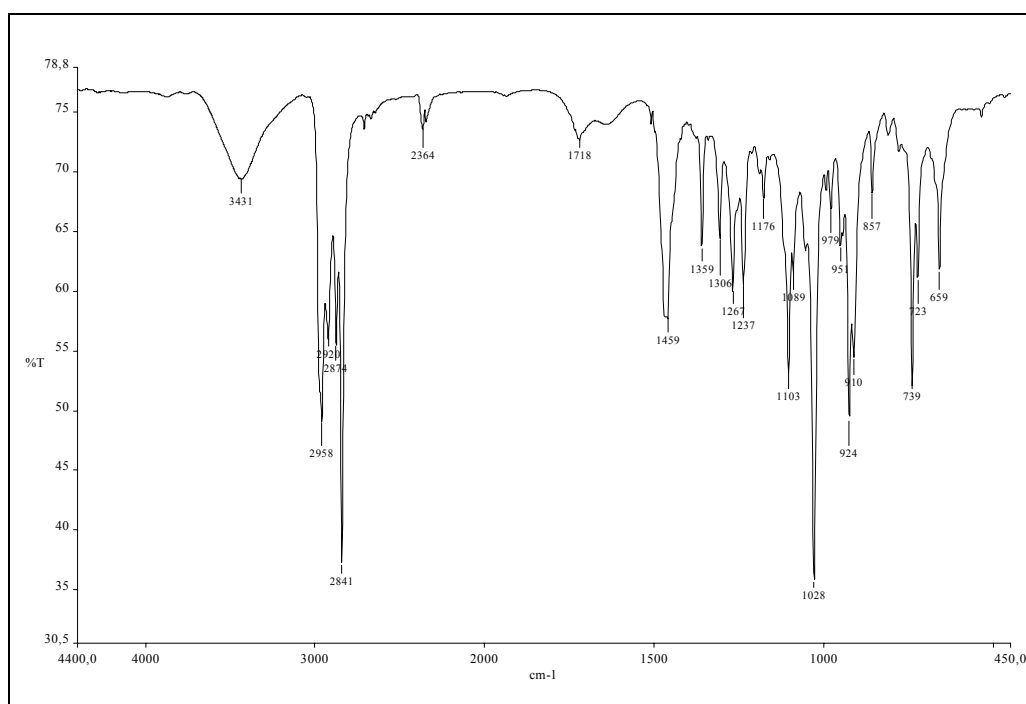
^1H - ^1H -NOESY



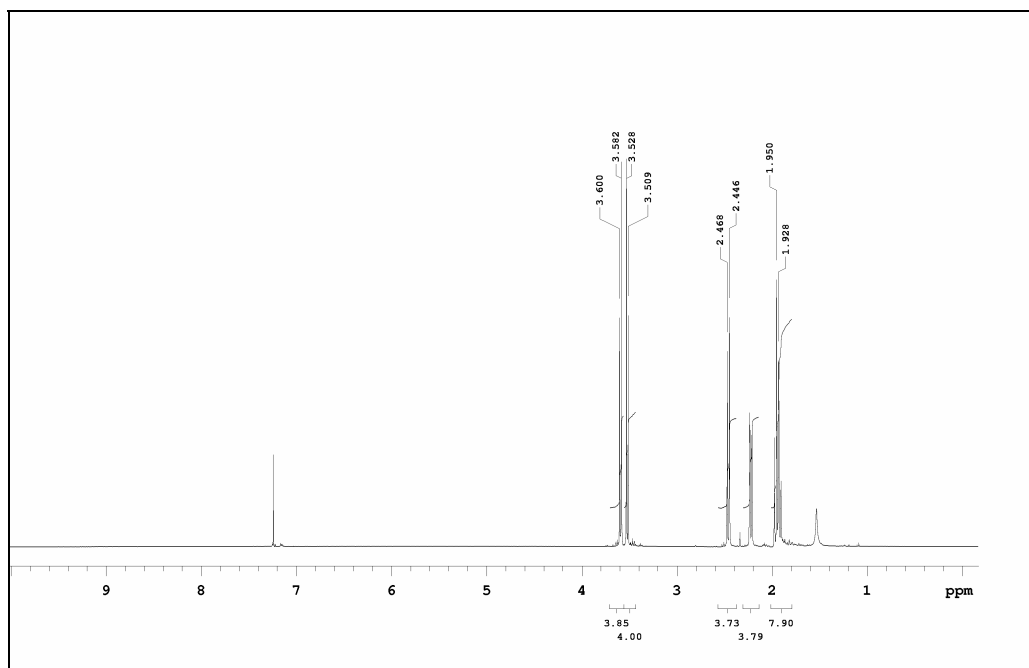
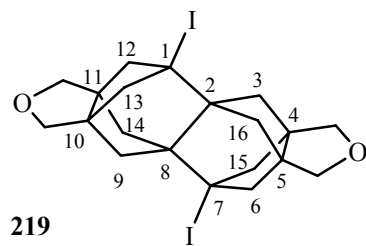
^1H - ^{13}C -HSQC



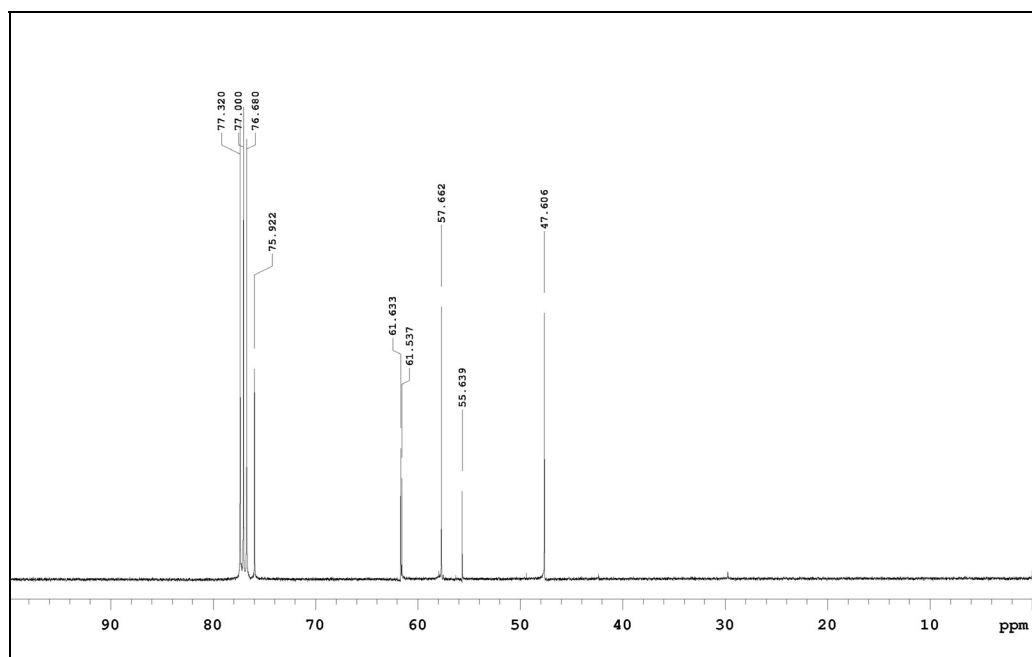
$^1\text{H}-^{13}\text{C}$ -HMBC $J = 8 \text{ Hz}$



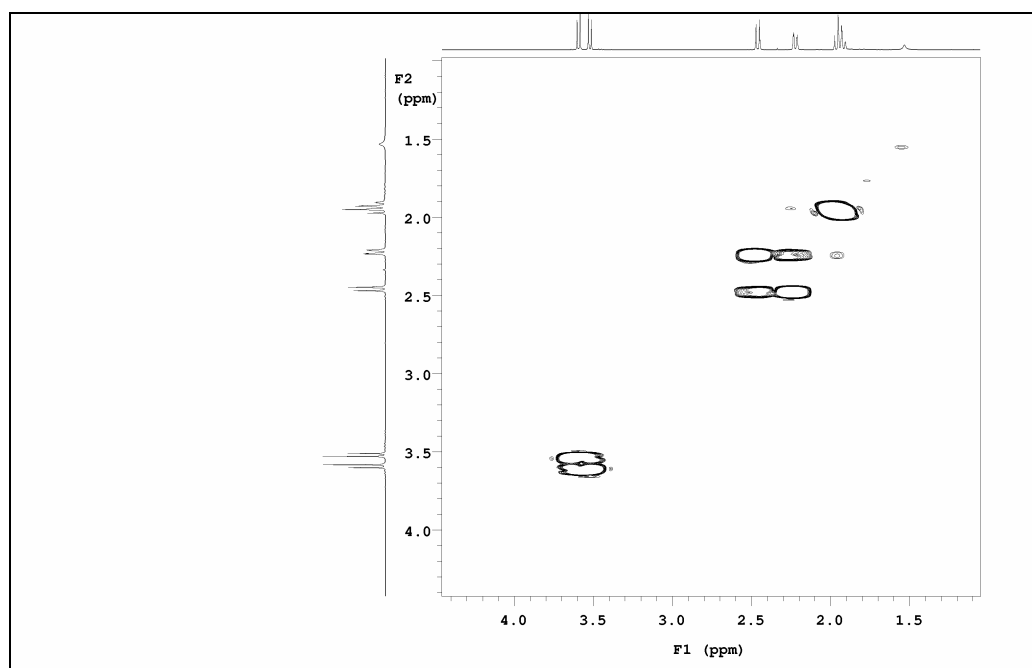
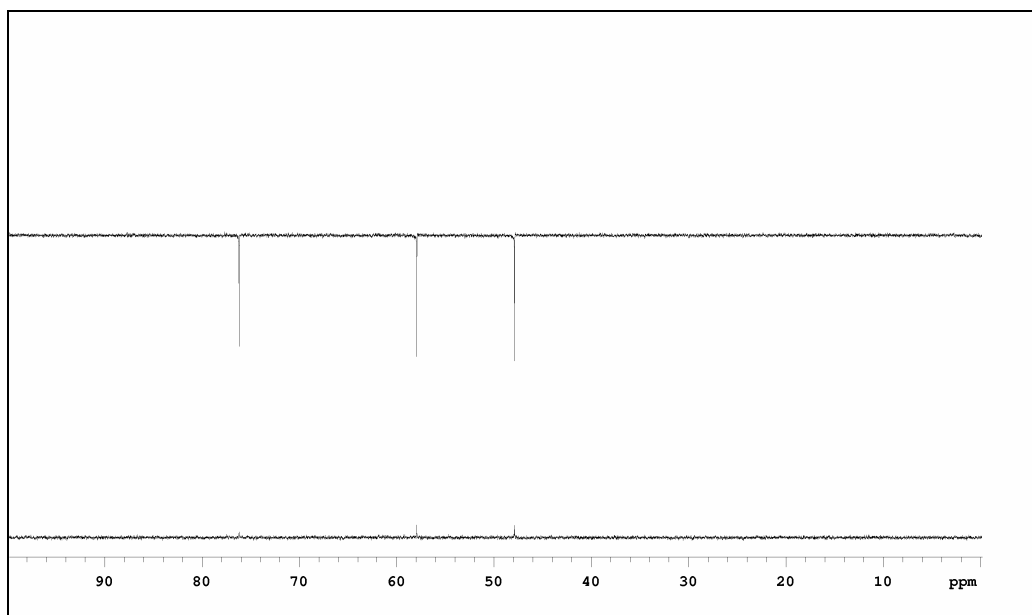
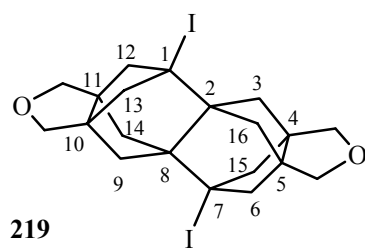
IR (KBr)

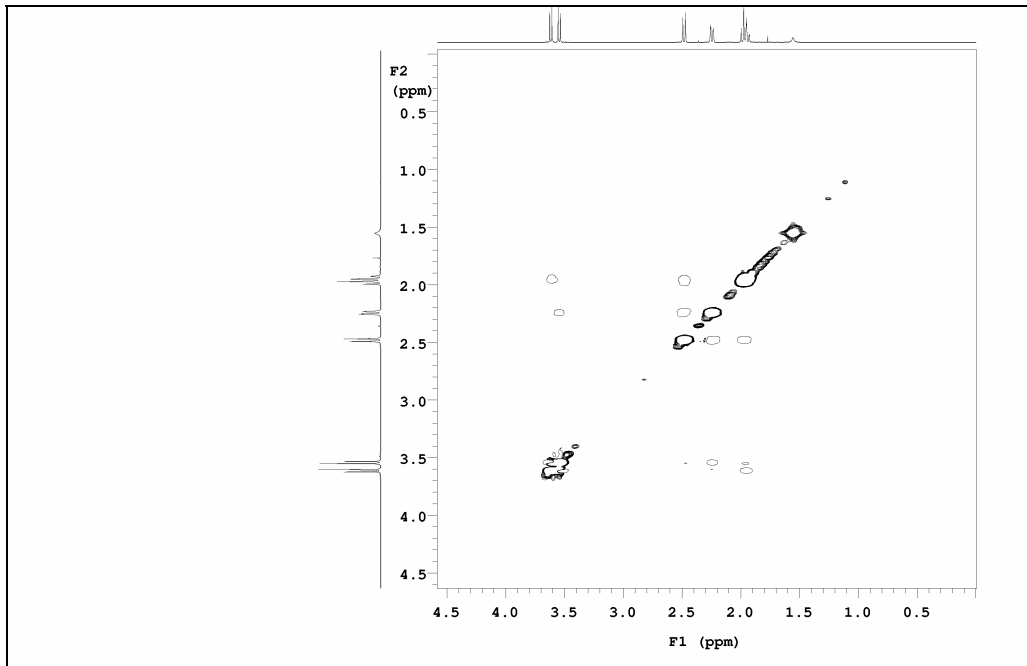
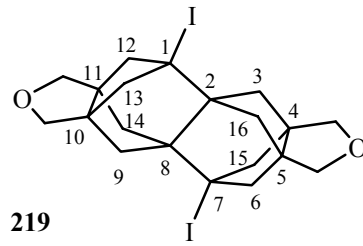


$^1\text{H-RMN}$ (500 MHz, CDCl_3)

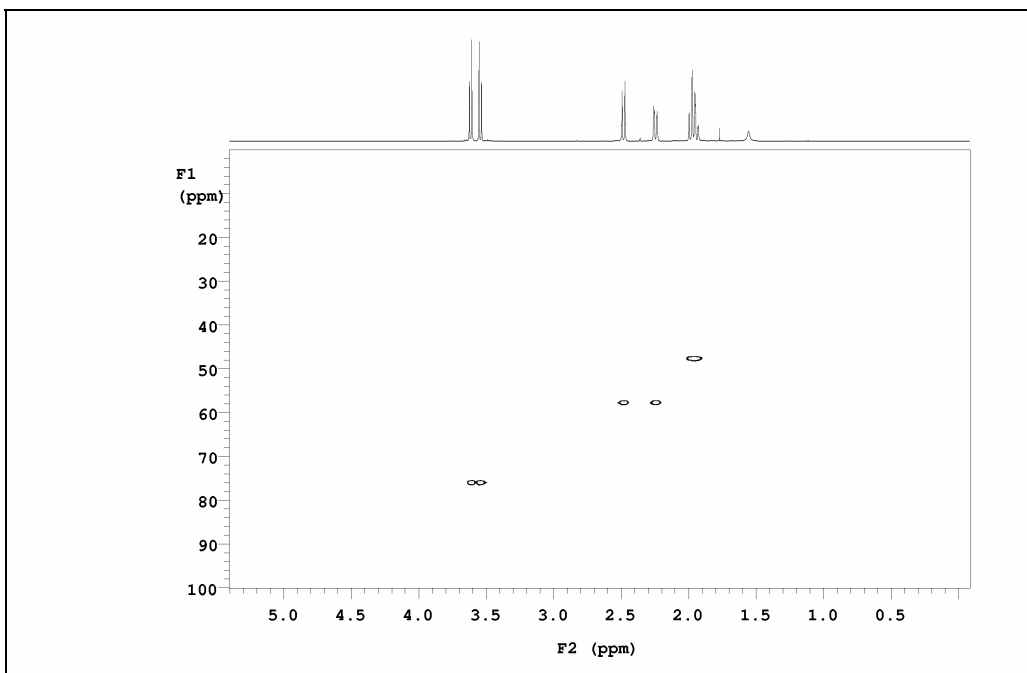


$^{13}\text{C-RMN}$ (100.6 MHz, CDCl_3)

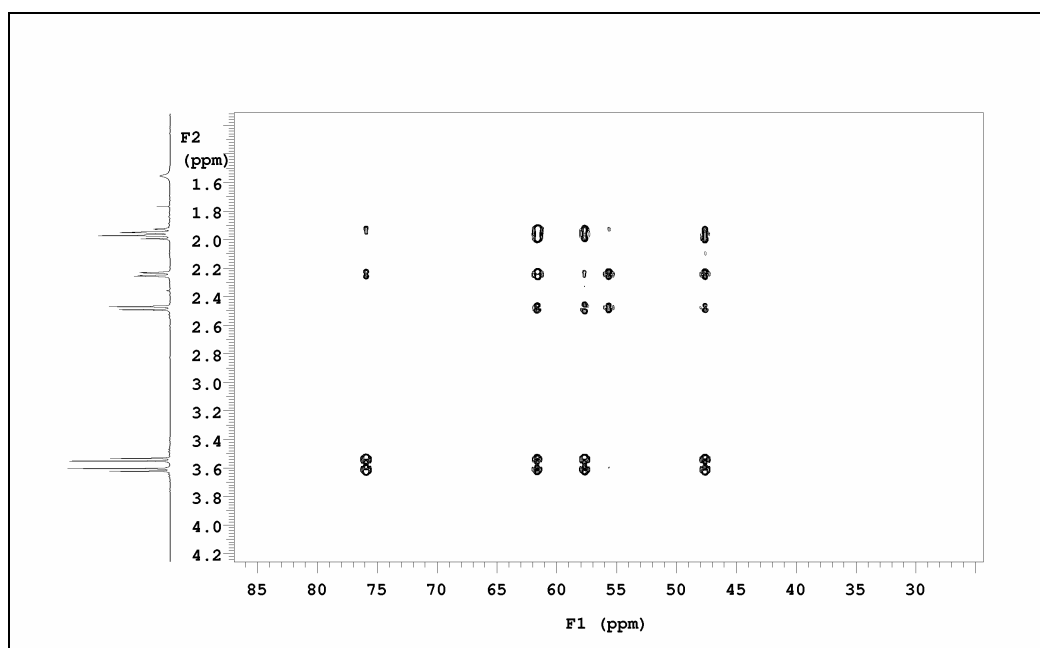
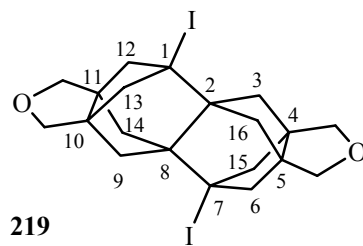




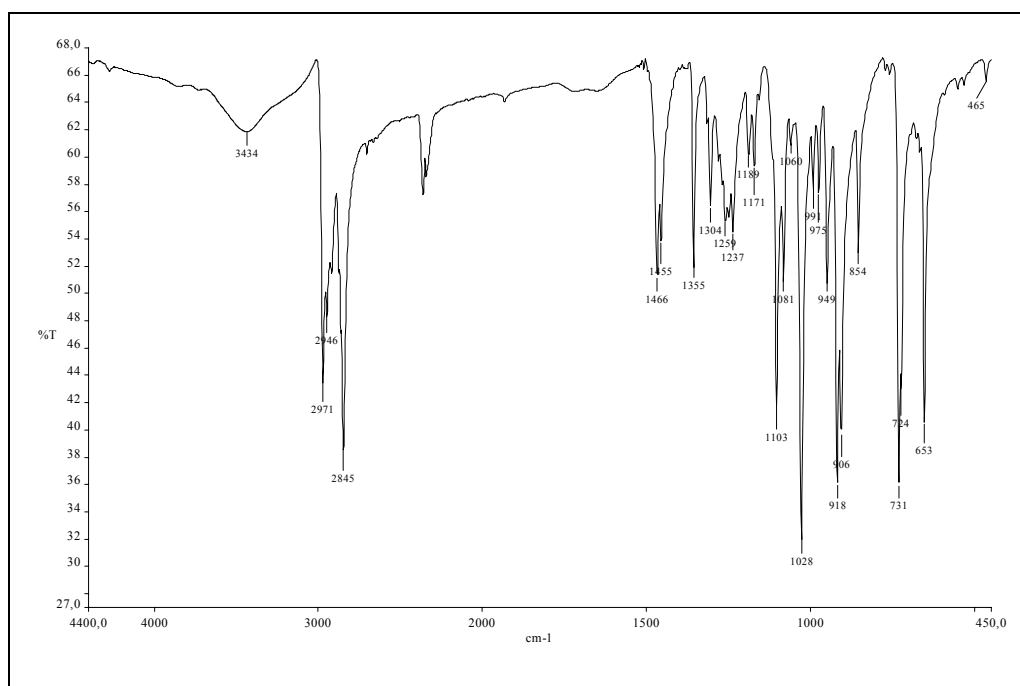
^1H - ^1H -NOESY



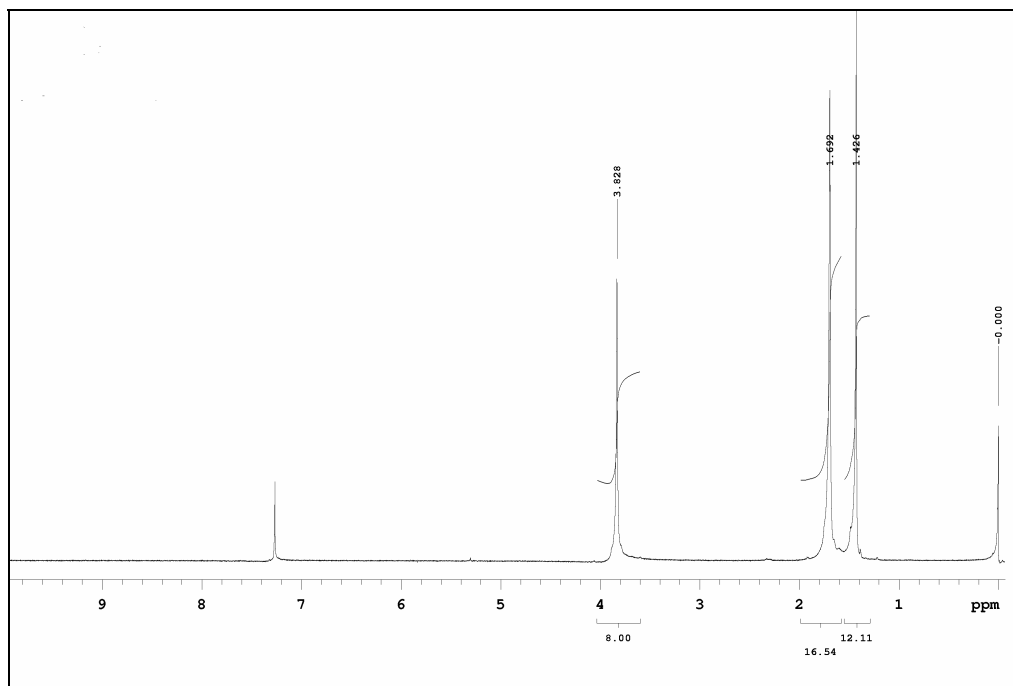
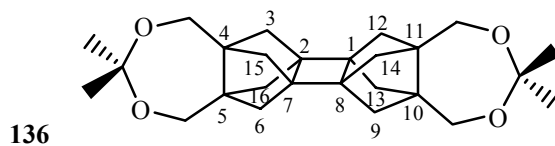
^1H - ^{13}C -HSQC



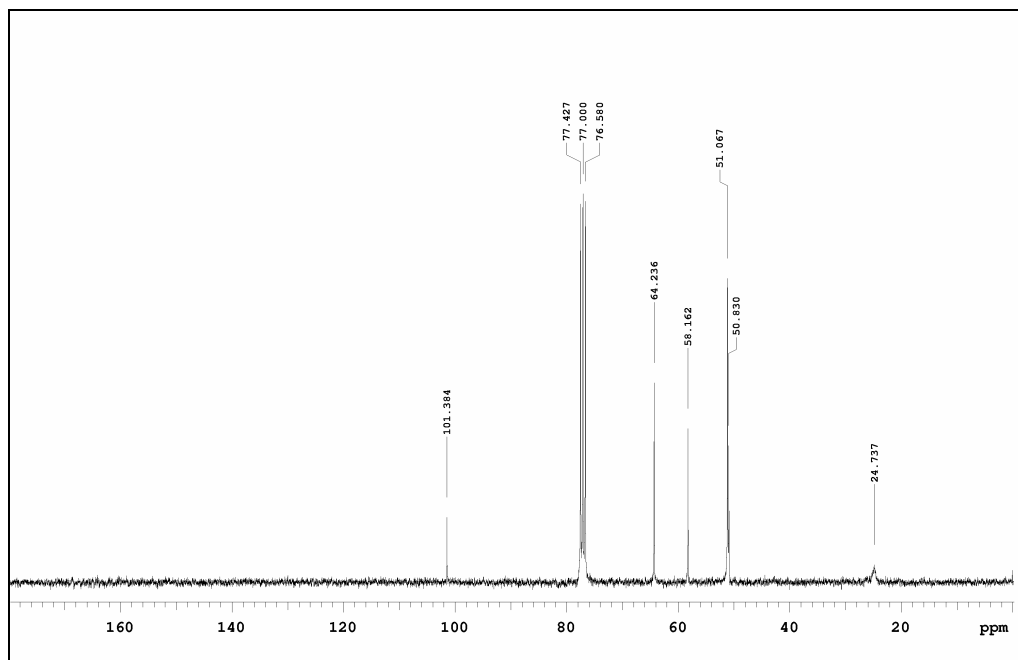
$^1\text{H}-^{13}\text{C}\text{-HMBC } J = 8\text{Hz}$



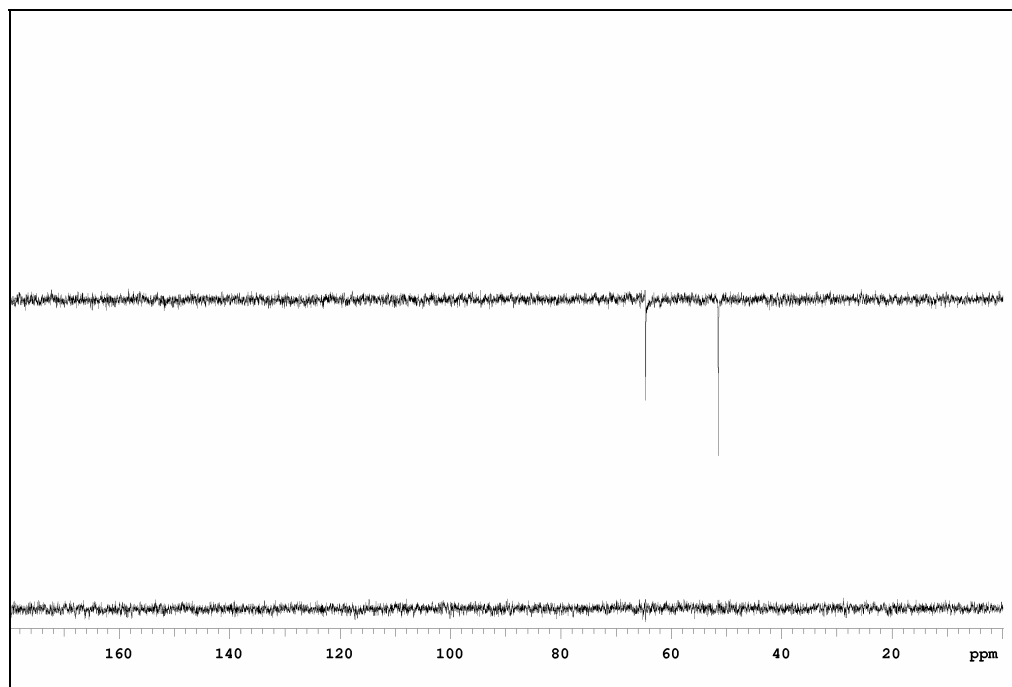
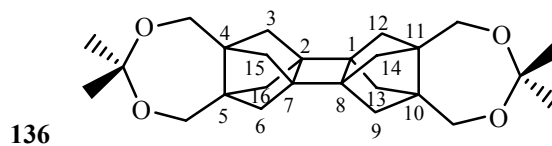
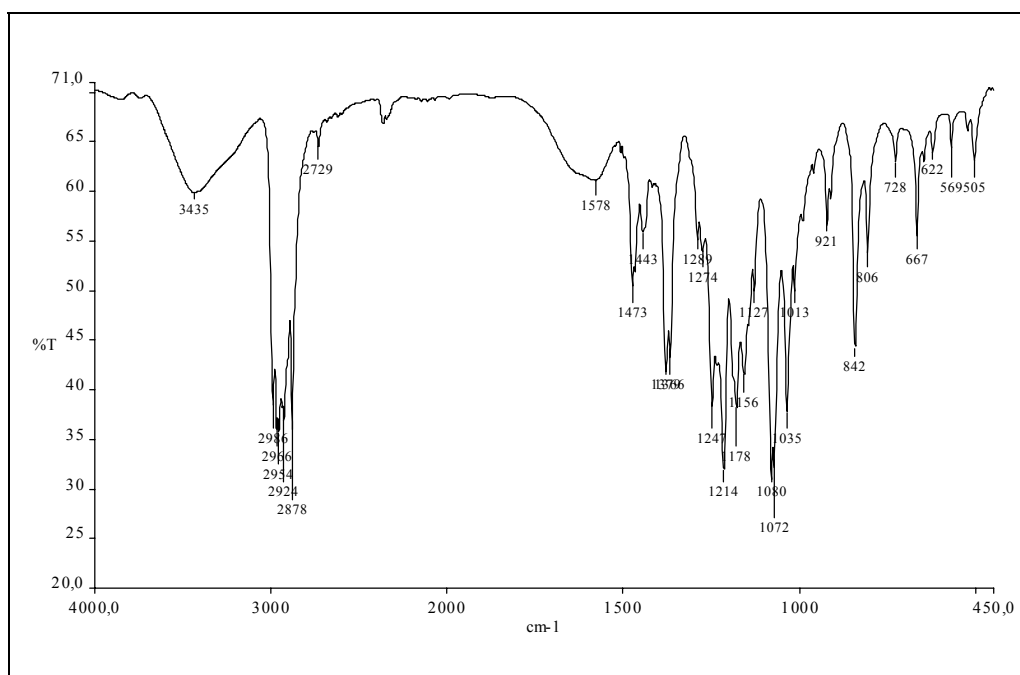
IR (KBr)



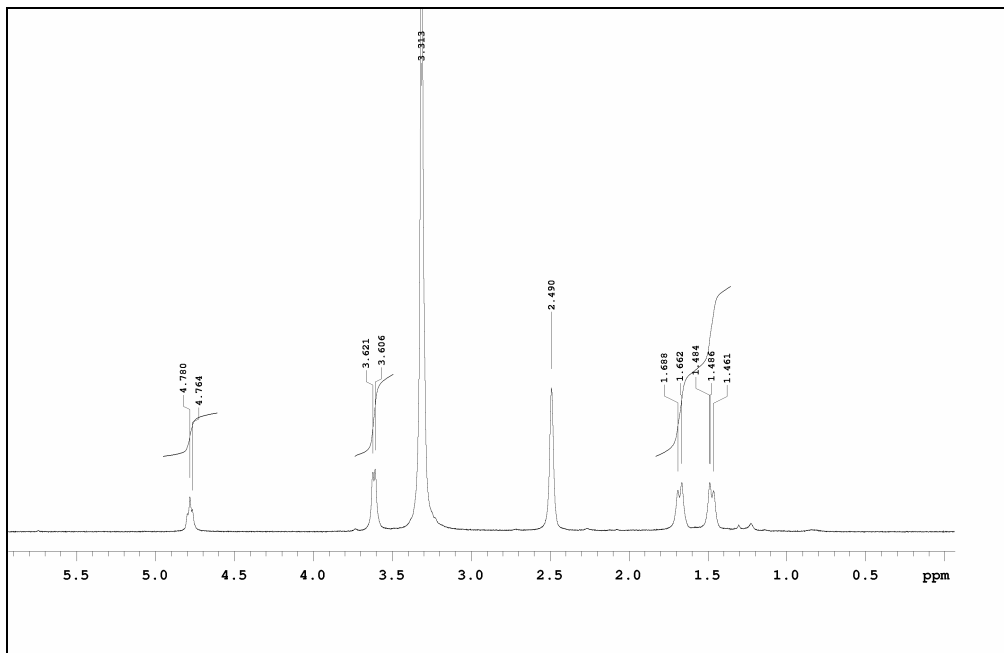
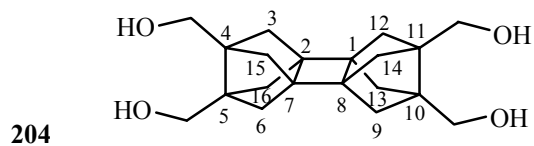
$^1\text{H-RMN}$ (300 MHz, CDCl_3)



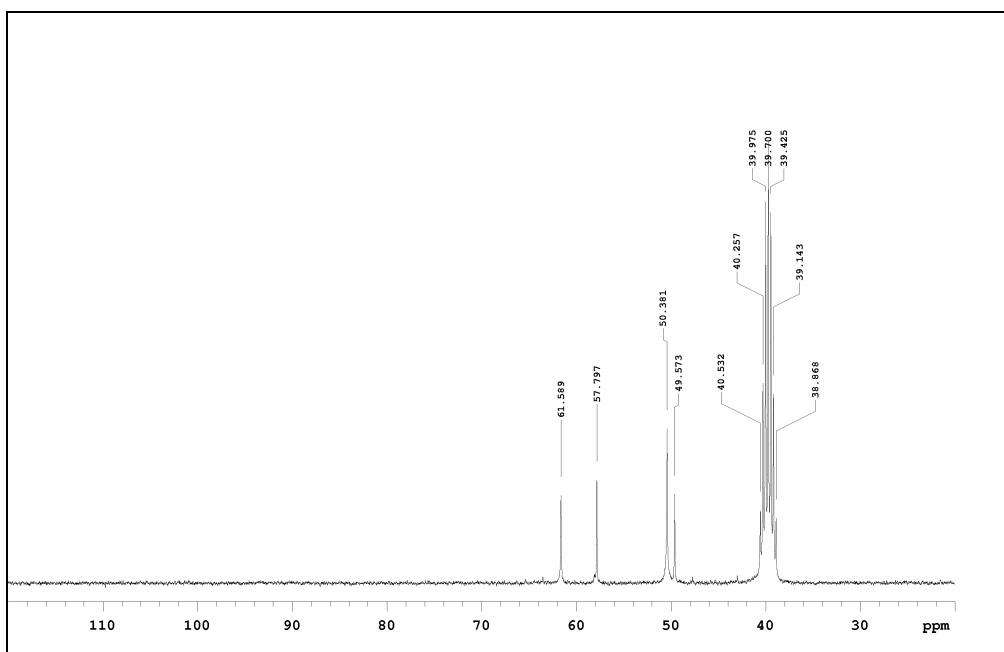
$^{13}\text{C-RMN}$ (75.4 MHz, CDCl_3)

¹³C-DEPT

IR (KBr)

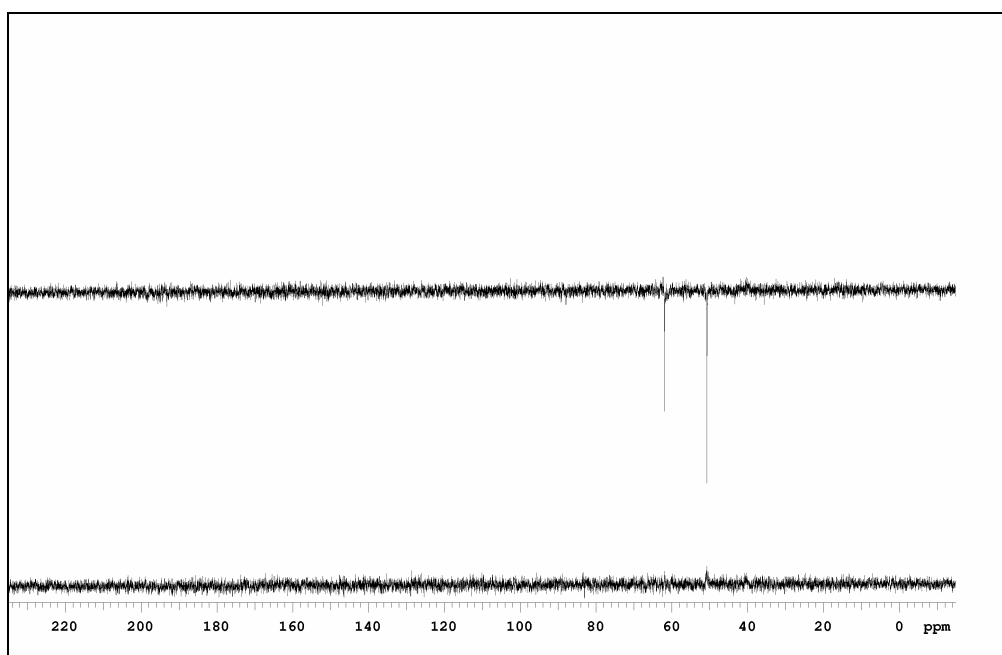
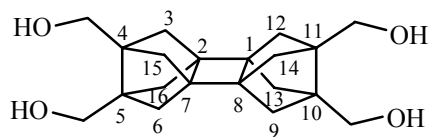
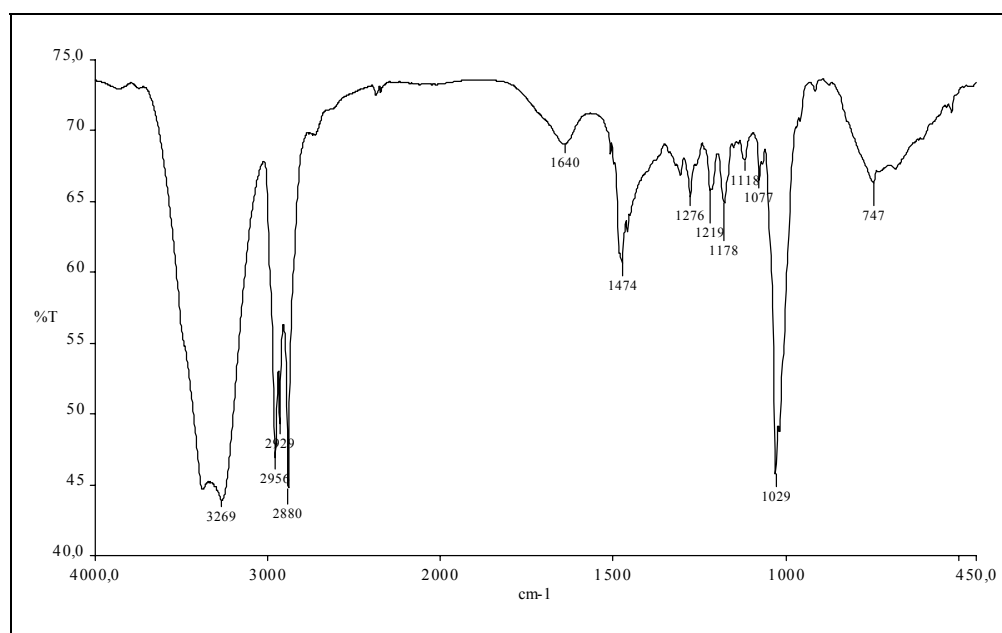


$^1\text{H-RMN}$ (300 MHz, DMSO-d_6)

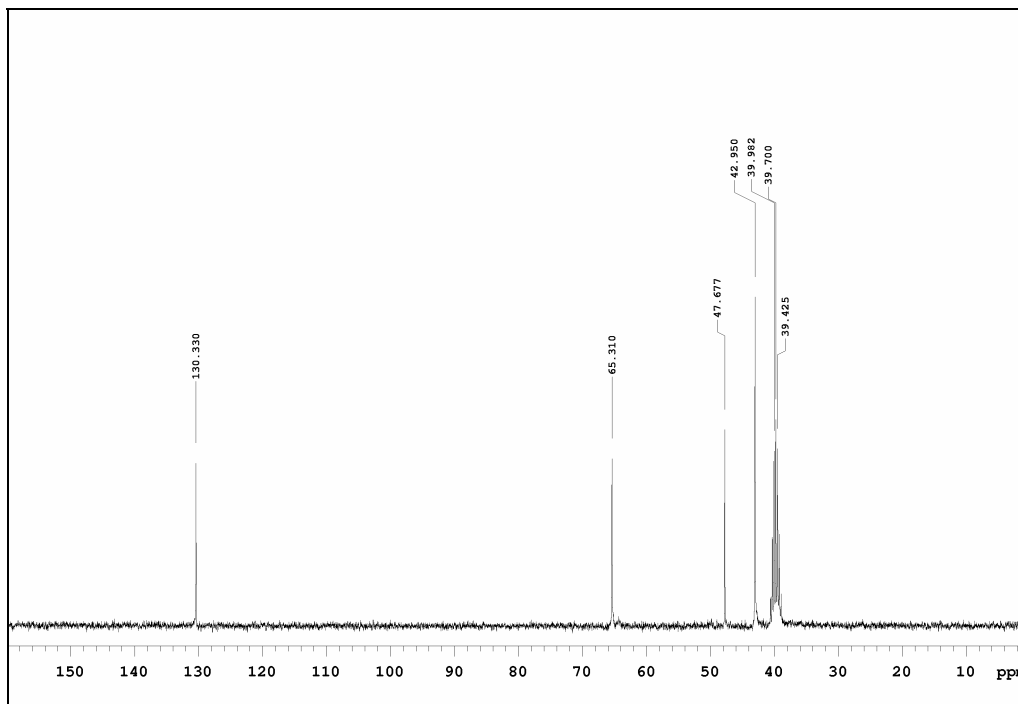
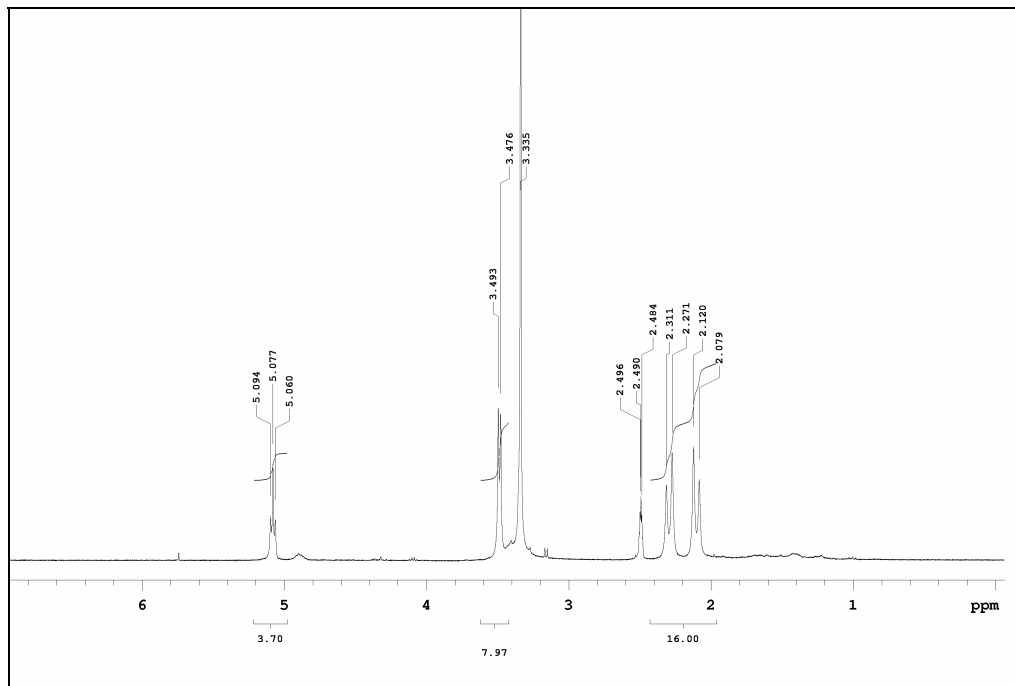
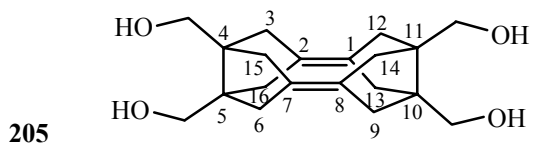


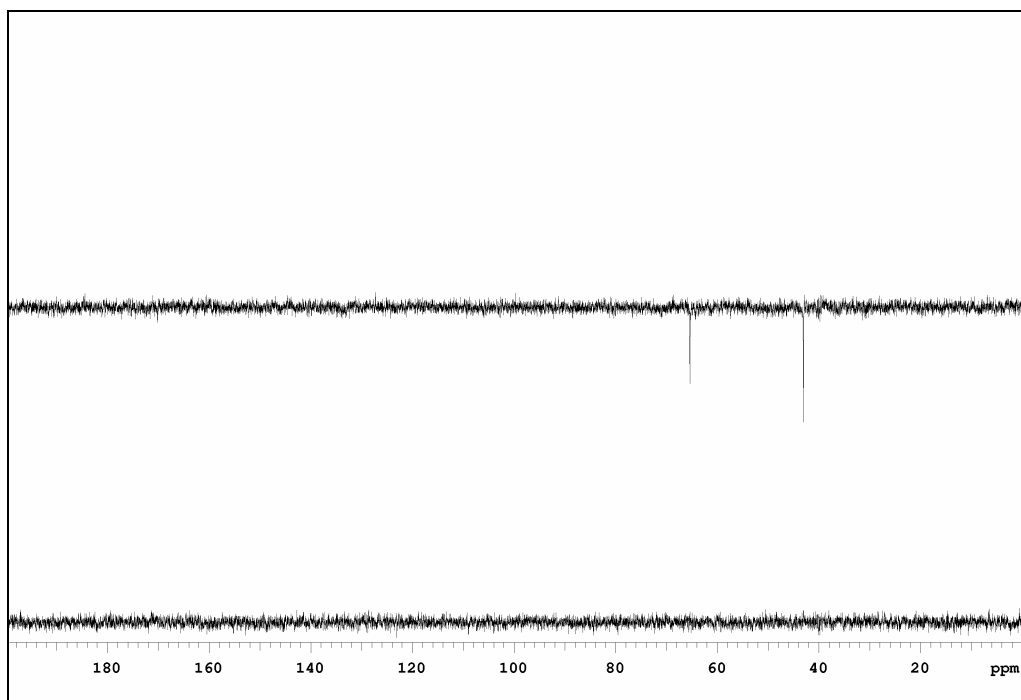
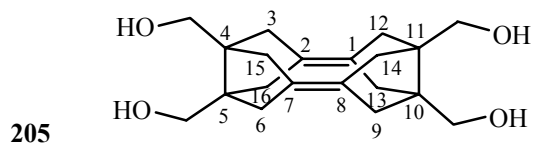
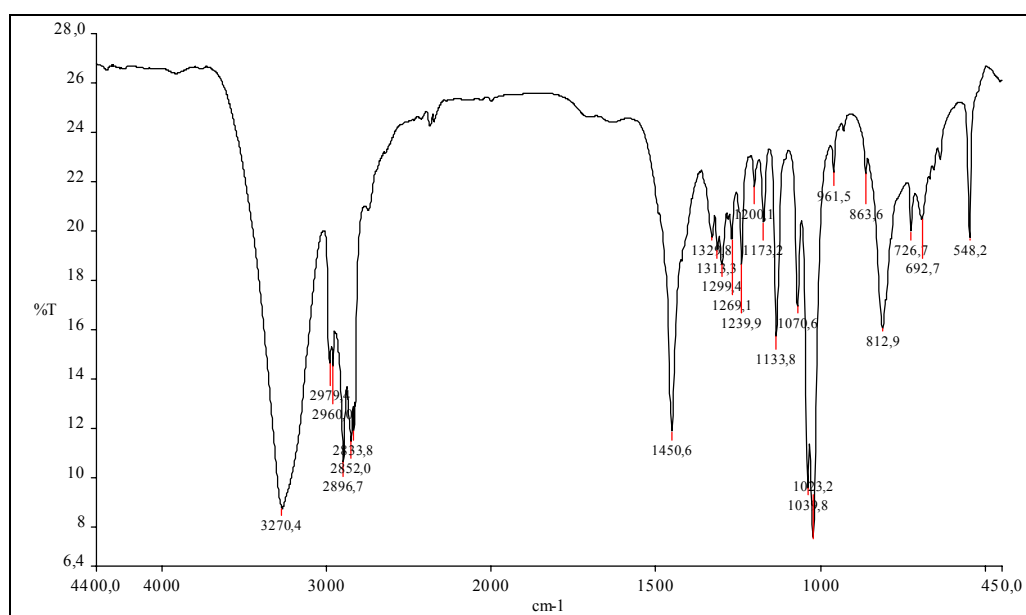
$^{13}\text{C-RMN}$ (75.4 MHz, DMSO_6)

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¹³C-DEPT

IR (KBr)

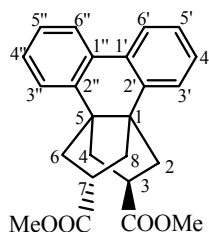


¹³C-DEPT

IR (KBr)

Anexo 2.

Rayos-X de endo,endo-105

R-X de endo,endo-105.

PCHM26

Experimental. A prismatic crystal (0.1x0.1x0.2 mm) was selected and mounted on a MNAR345 diffractometer with a image plate detector. Unit-cell parameters were determined from 10092 reflections ($3 < \theta < 31^\circ$) and refined by least-squares method. Intensities were collected with graphite monochromatized Mo $K\alpha$ radiation. 13970 reflections were measured in the range $2.95 \leq \theta \leq 31.61$. 5125 of which were non-equivalent by symmetry ($R_{int}(on I) = 0.022$). 4084 reflections were assumed as observed applying the condition $I > 2\sigma(I)$. Lorentz-polarization but no absorption corrections were made.

The structure was solved by Direct methods, using SHELXS computer program (Sheldrick, G.M., (1997), A computer program for determination of crystal structure Univer Göttingen, Germany) and refined by full-matrix least-squares method with SHELX97 computer program (Sheldrick, G.M., (1997), A computer program for determination of crystal structure. Univer Göttingen, Germany), using 5125 reflections, (very negative intensities were not assumed). The function minimized was $\sum w ||F_o|^2 - |F_c|^2|^2$, where $w = [\sigma^2(I) + (0.0677 P)^2 + 0.4756P]^{-1}$, and $P = (|F_o|^2 + 2 |F_c|^2)/3$, f , f' and f'' were taken from International Tables of X-Ray Crystallography (International Tables of X-Ray Crystallography, (1974), Ed. Kynoch press, Vol. IV, pp 99-100 and 149). All H atoms were located from a difference synthesis and refined with an overall isotropic temperature factor. The final $R(on F)$ factor was 0.055, $wR(on |F|^2) = 0.142$ and goodness of fit = 1.075 for all observed reflections. Number of refined parameters was 349. Max. shift/esd = 0.00, Mean shift/esd = 0.00. Max. and min. peaks in final difference synthesis was 0.251 and -0.176 $e\text{\AA}^{-3}$, respectively.

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Table 1. Crystal data and structure refinement for pchm26.

| | |
|-----------------------------------|---|
| Identification code | pchm26 |
| Empirical formula | C ₂₄ H ₂₄ O ₄ |
| Formula weight | 376.43 |
| Temperature | 293(2) K |
| Wavelength | 0.71069 Å |
| Crystal system, space group | Monoclinic, P2 ₁ /c |
| Unit cell dimensions | a = 9.3560(10) Å α = 90 °. b = 13.7910(10) Å β = 109.8580(10) °. c = 15.6330(10) Å γ = 90 °. |
| Volume | 1897.2(3) Å ³ |
| Z, Calculated density | 4, 1.318 Mg/m ³ |
| Absorption coefficient | 0.089 mm ⁻¹ |
| F(000) | 800 |
| Crystal size | 0.1 x 0.1 x 0.2 mm |
| Theta range for data collection | 2.95 to 31.61 °. |
| Index ranges | 0<=h<=13, -19<=k<=18, -22<=l<=21 |
| Reflections collected / unique | 13970 / 5125 [R(int) = 0.0229] |
| Refinement method | Full-matrix least-squares on F ² |
| Data / restraints / parameters | 5125 / 0 / 349 |
| Goodness-of-fit on F ² | 1.075 |
| Final R indices [I>2σ(I)] | R1 = 0.0558, wR2 = 0.1425 |
| R indices (all data) | R1 = 0.0723, wR2 = 0.1538 |
| Largest diff. peak and hole | 0.251 and -0.176 e.Å ⁻³ |

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for pchm26. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|---------|---------|-------|
| O(1) | 3422(2) | 8355(1) | 1819(1) | 79(1) |
| O(2) | 1270(1) | 8953(1) | 864(1) | 57(1) |
| O(3) | 3393(2) | 7181(1) | 4693(1) | 74(1) |
| O(4) | 5447(1) | 6295(1) | 4861(1) | 63(1) |
| C(1) | 520(2) | 3320(1) | 1129(1) | 50(1) |
| C(2) | 1787(3) | 2819(1) | 1135(1) | 61(1) |
| C(3) | 3190(2) | 3243(1) | 1478(1) | 63(1) |
| C(4) | 3313(2) | 4182(1) | 1804(1) | 52(1) |
| C(5) | 2045(2) | 4712(1) | 1794(1) | 38(1) |
| C(6) | 614(2) | 4268(1) | 1455(1) | 39(1) |
| C(7) | -757(2) | 4799(1) | 1457(1) | 40(1) |
| C(8) | -2204(2) | 4412(1) | 1026(1) | 53(1) |
| C(9) | -3482(2) | 4872(2) | 1071(1) | 61(1) |
| C(10) | -3351(2) | 5731(2) | 1541(1) | 60(1) |
| C(11) | -1937(2) | 6135(1) | 1954(1) | 50(1) |
| C(12) | -626(2) | 5681(1) | 1916(1) | 38(1) |
| C(13) | 911(2) | 6113(1) | 2421(1) | 35(1) |
| C(14) | 2174(2) | 5769(1) | 2062(1) | 36(1) |
| C(15) | 1996(2) | 6417(1) | 1229(1) | 43(1) |
| C(16) | 1204(2) | 7350(1) | 1372(1) | 41(1) |
| C(17) | 955(2) | 7215(1) | 2292(1) | 42(1) |
| C(18) | 1478(2) | 5807(1) | 3428(1) | 43(1) |
| C(19) | 3213(2) | 5793(1) | 3730(1) | 41(1) |
| C(20) | 3614(2) | 6011(1) | 2866(1) | 45(1) |
| C(21) | 2108(2) | 8257(1) | 1386(1) | 47(1) |
| C(22) | 2040(3) | 9856(2) | 865(2) | 72(1) |
| C(23) | 3981(2) | 6504(1) | 4471(1) | 45(1) |
| C(24) | 6307(3) | 6939(2) | 5578(2) | 78(1) |

Table 3. Bond lengths [Å] and angles [°] for pchm26.

| | |
|-------------------|------------|
| O(1)-C(21) | 1.193(2) |
| O(2)-C(21) | 1.3284(19) |
| O(2)-C(22) | 1.438(2) |
| O(3)-C(23) | 1.1930(19) |
| O(4)-C(23) | 1.3295(19) |
| O(4)-C(24) | 1.443(2) |
| C(1)-C(2) | 1.369(3) |
| C(1)-C(6) | 1.396(2) |
| C(2)-C(3) | 1.369(3) |
| C(3)-C(4) | 1.382(3) |
| C(4)-C(5) | 1.389(2) |
| C(5)-C(6) | 1.403(2) |
| C(5)-C(14) | 1.5093(19) |
| C(6)-C(7) | 1.477(2) |
| C(7)-C(8) | 1.397(2) |
| C(7)-C(12) | 1.398(2) |
| C(8)-C(9) | 1.376(3) |
| C(9)-C(10) | 1.377(3) |
| C(10)-C(11) | 1.377(3) |
| C(11)-C(12) | 1.396(2) |
| C(12)-C(13) | 1.5078(19) |
| C(13)-C(17) | 1.535(2) |
| C(13)-C(18) | 1.5399(17) |
| C(13)-C(14) | 1.5460(18) |
| C(14)-C(20) | 1.5352(19) |
| C(14)-C(15) | 1.5407(18) |
| C(15)-C(16) | 1.539(2) |
| C(16)-C(21) | 1.506(2) |
| C(16)-C(17) | 1.5451(19) |
| C(18)-C(19) | 1.529(2) |
| C(19)-C(23) | 1.5013(19) |
| C(19)-C(20) | 1.549(2) |
| C(21)-O(2)-C(22) | 115.70(16) |
| C(23)-O(4)-C(24) | 116.06(17) |
| C(2)-C(1)-C(6) | 121.56(17) |
| C(2)-C(3)-C(4) | 119.55(17) |
| C(3)-C(2)-C(1) | 120.02(17) |
| C(3)-C(4)-C(5) | 121.67(17) |
| C(4)-C(5)-C(6) | 118.49(14) |
| C(4)-C(5)-C(14) | 121.15(13) |
| C(6)-C(5)-C(14) | 120.13(12) |
| C(1)-C(6)-C(5) | 118.70(14) |
| C(1)-C(6)-C(7) | 121.20(14) |
| C(5)-C(6)-C(7) | 120.09(12) |
| C(8)-C(7)-C(12) | 118.76(14) |
| C(8)-C(7)-C(6) | 120.69(14) |
| C(12)-C(7)-C(6) | 120.52(12) |
| C(9)-C(8)-C(7) | 121.12(17) |
| C(8)-C(9)-C(10) | 120.11(16) |
| C(11)-C(10)-C(9) | 119.68(17) |
| C(10)-C(11)-C(12) | 121.15(17) |
| C(11)-C(12)-C(7) | 119.14(14) |
| C(11)-C(12)-C(13) | 119.77(14) |
| C(7)-C(12)-C(13) | 120.96(12) |
| C(12)-C(13)-C(17) | 112.68(12) |
| C(12)-C(13)-C(18) | 111.29(11) |

| | |
|-------------------|------------|
| C(17)-C(13)-C(18) | 112.95(11) |
| C(12)-C(13)-C(14) | 113.53(10) |
| C(17)-C(13)-C(14) | 101.46(10) |
| C(18)-C(13)-C(14) | 104.29(11) |
| C(5)-C(14)-C(20) | 113.73(12) |
| C(5)-C(14)-C(15) | 110.52(10) |
| C(20)-C(14)-C(15) | 112.25(12) |
| C(5)-C(14)-C(13) | 113.48(11) |
| C(20)-C(14)-C(13) | 101.65(10) |
| C(15)-C(14)-C(13) | 104.60(11) |
| C(16)-C(15)-C(14) | 106.38(11) |
| C(21)-C(16)-C(15) | 113.69(13) |
| C(21)-C(16)-C(17) | 110.39(12) |
| C(15)-C(16)-C(17) | 105.45(11) |
| C(13)-C(17)-C(16) | 105.13(11) |
| C(19)-C(18)-C(13) | 106.26(11) |
| C(23)-C(19)-C(18) | 114.13(13) |
| C(23)-C(19)-C(20) | 110.60(12) |
| C(18)-C(19)-C(20) | 105.95(11) |
| C(14)-C(20)-C(19) | 105.47(11) |
| O(1)-C(21)-O(2) | 123.07(15) |
| O(1)-C(21)-C(16) | 124.60(15) |
| O(2)-C(21)-C(16) | 112.32(13) |
| O(3)-C(23)-O(4) | 122.78(14) |
| O(3)-C(23)-C(19) | 126.06(15) |
| O(4)-C(23)-C(19) | 111.15(13) |

Symmetry transformations used to generate equivalent atoms:

Table 4. Hydrogen bond lengths [Å] and angles [°] for pchm26.

| | |
|--------------------|-----------|
| C(1)-H(1) | 0.96(2) |
| C(2)-H(2) | 0.93(2) |
| C(3)-H(3) | 0.97(2) |
| C(4)-H(4) | 0.99(2) |
| C(8)-H(8) | 1.01(2) |
| C(9)-H(9) | 0.98(2) |
| C(10)-H(10) | 1.01(2) |
| C(11)-H(11) | 0.98(2) |
| C(15)-H(15) | 0.991(19) |
| C(15)-H(15A) | 0.993(19) |
| C(16)-H(16) | 0.964(18) |
| C(17)-H(17) | 0.972(19) |
| C(17)-H(17A) | 1.005(19) |
| C(18)-H(18) | 0.97(2) |
| C(18)-H(18A) | 1.003(19) |
| C(19)-H(19) | 0.978(17) |
| C(20)-H(20) | 1.03(2) |
| C(20)-H(20A) | 0.998(19) |
| C(22)-H(22) | 1.01(3) |
| C(22)-H(22A) | 0.96(3) |
| C(22)-H(22B) | 1.03(4) |
| C(24)-H(24) | 0.97(3) |
| C(24)-H(24A) | 0.99(3) |
| C(24)-H(24B) | 0.97(3) |
| | |
| C(2)-C(1)-H(1) | 119.0(12) |
| C(6)-C(1)-H(1) | 119.4(12) |
| C(3)-C(2)-H(2) | 121.5(14) |
| C(1)-C(2)-H(2) | 118.4(14) |
| C(2)-C(3)-H(3) | 121.3(14) |
| C(4)-C(3)-H(3) | 119.1(15) |
| C(3)-C(4)-H(4) | 119.3(13) |
| C(5)-C(4)-H(4) | 119.0(13) |
| C(9)-C(8)-H(8) | 119.8(12) |
| C(7)-C(8)-H(8) | 119.1(12) |
| C(8)-C(9)-H(9) | 119.2(13) |
| C(10)-C(9)-H(9) | 120.6(13) |
| C(11)-C(10)-H(10) | 120.0(13) |
| C(9)-C(10)-H(10) | 120.4(13) |
| C(10)-C(11)-H(11) | 120.8(11) |
| C(12)-C(11)-H(11) | 118.1(11) |
| C(16)-C(15)-H(15) | 109.2(10) |
| C(14)-C(15)-H(15) | 109.9(10) |
| C(16)-C(15)-H(15A) | 113.0(11) |
| C(14)-C(15)-H(15A) | 110.4(11) |
| H(15)-C(15)-H(15A) | 108.0(15) |
| C(21)-C(16)-H(16) | 108.7(10) |
| C(15)-C(16)-H(16) | 109.2(10) |
| C(17)-C(16)-H(16) | 109.3(10) |
| C(13)-C(17)-H(17) | 112.9(11) |
| C(16)-C(17)-H(17) | 112.0(10) |
| C(13)-C(17)-H(17A) | 111.1(10) |
| C(16)-C(17)-H(17A) | 110.3(10) |
| H(17)-C(17)-H(17A) | 105.6(15) |
| C(19)-C(18)-H(18) | 112.5(11) |
| C(13)-C(18)-H(18) | 110.9(11) |
| C(19)-C(18)-H(18A) | 110.7(10) |

| | |
|---------------------|-----------|
| C(13)-C(18)-H(18A) | 108.0(10) |
| H(18)-C(18)-H(18A) | 108.4(15) |
| C(23)-C(19)-H(19) | 106.3(9) |
| C(18)-C(19)-H(19) | 111.2(9) |
| C(20)-C(19)-H(19) | 108.6(9) |
| C(14)-C(20)-H(20) | 109.3(10) |
| C(19)-C(20)-H(20) | 111.7(10) |
| C(14)-C(20)-H(20A) | 113.3(11) |
| C(19)-C(20)-H(20A) | 111.4(11) |
| H(20)-C(20)-H(20A) | 105.8(15) |
| O(2)-C(22)-H(22) | 107.2(16) |
| O(2)-C(22)-H(22A) | 108.2(16) |
| H(22)-C(22)-H(22A) | 97(2) |
| O(2)-C(22)-H(22B) | 105.2(19) |
| H(22)-C(22)-H(22B) | 122(2) |
| H(22A)-C(22)-H(22B) | 116(3) |
| O(4)-C(24)-H(24) | 108.4(16) |
| O(4)-C(24)-H(24A) | 109.6(18) |
| H(24)-C(24)-H(24A) | 109(2) |
| O(4)-C(24)-H(24B) | 108.1(19) |
| H(24)-C(24)-H(24B) | 112(2) |
| H(24A)-C(24)-H(24B) | 110(2) |

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for pchm26.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

| | U_{11} | U_{22} | U_{33} | U_{23} | U_{13} | U_{12} |
|-------|----------|----------|----------|----------|----------|----------|
| O(1) | 56(1) | 75(1) | 85(1) | 14(1) | -3(1) | -23(1) |
| O(2) | 63(1) | 42(1) | 62(1) | 7(1) | 17(1) | -5(1) |
| O(3) | 81(1) | 60(1) | 66(1) | -17(1) | 7(1) | 17(1) |
| O(4) | 50(1) | 60(1) | 61(1) | -17(1) | -3(1) | -1(1) |
| C(1) | 63(1) | 44(1) | 44(1) | -1(1) | 18(1) | -7(1) |
| C(2) | 87(1) | 41(1) | 58(1) | 0(1) | 28(1) | 7(1) |
| C(3) | 68(1) | 57(1) | 66(1) | -2(1) | 24(1) | 20(1) |
| C(4) | 45(1) | 56(1) | 55(1) | -2(1) | 17(1) | 11(1) |
| C(5) | 39(1) | 42(1) | 34(1) | 2(1) | 12(1) | 3(1) |
| C(6) | 43(1) | 42(1) | 32(1) | 2(1) | 13(1) | -2(1) |
| C(7) | 36(1) | 50(1) | 32(1) | 4(1) | 10(1) | -5(1) |
| C(8) | 43(1) | 67(1) | 44(1) | -1(1) | 10(1) | -15(1) |
| C(9) | 37(1) | 90(1) | 51(1) | 8(1) | 8(1) | -12(1) |
| C(10) | 35(1) | 85(1) | 61(1) | 19(1) | 17(1) | 6(1) |
| C(11) | 42(1) | 60(1) | 51(1) | 9(1) | 20(1) | 7(1) |
| C(12) | 34(1) | 47(1) | 33(1) | 8(1) | 12(1) | 2(1) |
| C(13) | 34(1) | 42(1) | 31(1) | 2(1) | 12(1) | 2(1) |
| C(14) | 32(1) | 42(1) | 33(1) | 0(1) | 11(1) | -1(1) |
| C(15) | 49(1) | 46(1) | 37(1) | 1(1) | 19(1) | -4(1) |
| C(16) | 42(1) | 43(1) | 37(1) | 3(1) | 10(1) | -4(1) |
| C(17) | 46(1) | 42(1) | 41(1) | -1(1) | 18(1) | 0(1) |
| C(18) | 44(1) | 52(1) | 33(1) | 3(1) | 13(1) | -2(1) |
| C(19) | 43(1) | 40(1) | 35(1) | 1(1) | 6(1) | 1(1) |
| C(20) | 34(1) | 59(1) | 40(1) | -6(1) | 10(1) | -4(1) |
| C(21) | 50(1) | 47(1) | 41(1) | 3(1) | 12(1) | -5(1) |
| C(22) | 96(2) | 43(1) | 76(1) | 2(1) | 28(1) | -16(1) |
| C(23) | 54(1) | 40(1) | 35(1) | 4(1) | 7(1) | 2(1) |
| C(24) | 74(2) | 76(2) | 64(1) | -20(1) | -2(1) | -20(1) |

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for pchm26.

| | x | y | z | U(eq) |
|--------|----------|----------|----------|---------|
| H(1) | -450(2) | 3001(15) | 916(13) | 56(5) |
| H(2) | 1670(2) | 2188(17) | 907(15) | 72(6) |
| H(3) | 4110(3) | 2900(18) | 1487(16) | 83(7) |
| H(4) | 4330(3) | 4485(17) | 2055(16) | 76(6) |
| H(8) | -2310(2) | 3774(17) | 689(15) | 72(6) |
| H(9) | -4490(2) | 4600(16) | 737(15) | 68(6) |
| H(10) | -4280(3) | 6059(17) | 1591(15) | 77(7) |
| H(11) | -1820(2) | 6745(15) | 2288(13) | 54(5) |
| H(15) | 1340(2) | 6088(13) | 668(13) | 49(5) |
| H(15A) | 3000(2) | 6540(14) | 1165(13) | 59(5) |
| H(16) | 230(2) | 7407(13) | 894(12) | 48(4) |
| H(17) | 40(2) | 7538(13) | 2303(12) | 52(5) |
| H(17A) | 1810(2) | 7519(13) | 2796(12) | 51(5) |
| H(18) | 1100(2) | 6247(14) | 3791(13) | 56(5) |
| H(18A) | 1073(19) | 5142(14) | 3469(12) | 49(5) |
| H(19) | 3617(17) | 5154(12) | 3960(11) | 39(4) |
| H(20) | 3890(2) | 6734(15) | 2831(12) | 56(5) |
| H(20A) | 4520(2) | 5637(14) | 2862(13) | 56(5) |
| H(22) | 3060(3) | 9690(2) | 814(19) | 101(9) |
| H(22A) | 2410(3) | 10100(2) | 1480(2) | 96(8) |
| H(22B) | 1260(4) | 10290(3) | 400(3) | 137(11) |
| H(24) | 6180(3) | 7600(2) | 5342(18) | 95(8) |
| H(24A) | 5920(3) | 6900(2) | 6090(2) | 111(10) |
| H(24B) | 7370(4) | 6740(2) | 5780(2) | 120(11) |

Table 8. Torsion angles [deg] for pchm26.

| | |
|-------------------------|-------------|
| C(6)-C(1)-C(2)-C(3) | 1.0(3) |
| C(1)-C(2)-C(3)-C(4) | -1.0(3) |
| C(2)-C(3)-C(4)-C(5) | 0.1(3) |
| C(3)-C(4)-C(5)-C(6) | 0.9(2) |
| C(3)-C(4)-C(5)-C(14) | -173.66(15) |
| C(2)-C(1)-C(6)-C(5) | 0.0(2) |
| C(2)-C(1)-C(6)-C(7) | -179.23(14) |
| C(4)-C(5)-C(6)-C(1) | -0.90(19) |
| C(14)-C(5)-C(6)-C(1) | 173.68(12) |
| C(4)-C(5)-C(6)-C(7) | 178.34(12) |
| C(14)-C(5)-C(6)-C(7) | -7.08(17) |
| C(1)-C(6)-C(7)-C(8) | -8.31(19) |
| C(5)-C(6)-C(7)-C(8) | 172.47(12) |
| C(1)-C(6)-C(7)-C(12) | 169.52(12) |
| C(5)-C(6)-C(7)-C(12) | -9.70(18) |
| C(12)-C(7)-C(8)-C(9) | -1.8(2) |
| C(6)-C(7)-C(8)-C(9) | 176.04(14) |
| C(7)-C(8)-C(9)-C(10) | 0.4(3) |
| C(8)-C(9)-C(10)-C(11) | 0.9(3) |
| C(9)-C(10)-C(11)-C(12) | -0.9(2) |
| C(10)-C(11)-C(12)-C(7) | -0.5(2) |
| C(10)-C(11)-C(12)-C(13) | -176.51(13) |
| C(8)-C(7)-C(12)-C(11) | 1.86(19) |
| C(6)-C(7)-C(12)-C(11) | -176.01(12) |
| C(8)-C(7)-C(12)-C(13) | 177.78(12) |
| C(6)-C(7)-C(12)-C(13) | -0.09(18) |
| C(11)-C(12)-C(13)-C(17) | -45.01(16) |
| C(7)-C(12)-C(13)-C(17) | 139.10(12) |
| C(11)-C(12)-C(13)-C(18) | 83.05(16) |
| C(7)-C(12)-C(13)-C(18) | -92.84(14) |
| C(11)-C(12)-C(13)-C(14) | -159.65(12) |
| C(7)-C(12)-C(13)-C(14) | 24.45(16) |
| C(4)-C(5)-C(14)-C(20) | -38.77(17) |
| C(6)-C(5)-C(14)-C(20) | 146.79(12) |
| C(4)-C(5)-C(14)-C(15) | 88.53(16) |
| C(6)-C(5)-C(14)-C(15) | -85.90(14) |
| C(4)-C(5)-C(14)-C(13) | -154.33(13) |
| C(6)-C(5)-C(14)-C(13) | 31.23(16) |
| C(12)-C(13)-C(14)-C(5) | -38.57(14) |
| C(17)-C(13)-C(14)-C(5) | -159.73(11) |
| C(18)-C(13)-C(14)-C(5) | 82.74(13) |
| C(12)-C(13)-C(14)-C(20) | -161.09(11) |
| C(17)-C(13)-C(14)-C(20) | 77.75(12) |
| C(18)-C(13)-C(14)-C(20) | -39.78(14) |
| C(12)-C(13)-C(14)-C(15) | 81.97(13) |
| C(17)-C(13)-C(14)-C(15) | -39.19(13) |
| C(18)-C(13)-C(14)-C(15) | -156.73(11) |
| C(5)-C(14)-C(15)-C(16) | 146.81(12) |
| C(20)-C(14)-C(15)-C(16) | -85.07(14) |
| C(13)-C(14)-C(15)-C(16) | 24.32(14) |
| C(14)-C(15)-C(16)-C(21) | 121.35(12) |
| C(14)-C(15)-C(16)-C(17) | 0.29(15) |
| C(12)-C(13)-C(17)-C(16) | -82.17(14) |
| C(18)-C(13)-C(17)-C(16) | 150.64(12) |
| C(14)-C(13)-C(17)-C(16) | 39.58(14) |
| C(21)-C(16)-C(17)-C(13) | -148.24(12) |
| C(15)-C(16)-C(17)-C(13) | -25.05(15) |

| | |
|-------------------------|-------------|
| C(12)-C(13)-C(18)-C(19) | 150.47(12) |
| C(17)-C(13)-C(18)-C(19) | -81.62(15) |
| C(14)-C(13)-C(18)-C(19) | 27.68(15) |
| C(13)-C(18)-C(19)-C(23) | 117.47(13) |
| C(13)-C(18)-C(19)-C(20) | -4.47(16) |
| C(5)-C(14)-C(20)-C(19) | -85.21(14) |
| C(15)-C(14)-C(20)-C(19) | 148.39(12) |
| C(13)-C(14)-C(20)-C(19) | 37.14(14) |
| C(23)-C(19)-C(20)-C(14) | -144.79(13) |
| C(18)-C(19)-C(20)-C(14) | -20.62(16) |
| C(22)-O(2)-C(21)-O(1) | -1.3(3) |
| C(22)-O(2)-C(21)-C(16) | 178.01(15) |
| C(15)-C(16)-C(21)-O(1) | -48.0(2) |
| C(17)-C(16)-C(21)-O(1) | 70.3(2) |
| C(15)-C(16)-C(21)-O(2) | 132.76(13) |
| C(17)-C(16)-C(21)-O(2) | -108.98(14) |
| C(24)-O(4)-C(23)-O(3) | 0.0(3) |
| C(24)-O(4)-C(23)-C(19) | 179.32(17) |
| C(18)-C(19)-C(23)-O(3) | -16.7(2) |
| C(20)-C(19)-C(23)-O(3) | 102.68(19) |
| C(18)-C(19)-C(23)-O(4) | 164.08(12) |
| C(20)-C(19)-C(23)-O(4) | -76.57(16) |

Symmetry transformations used to generate equivalent atoms:

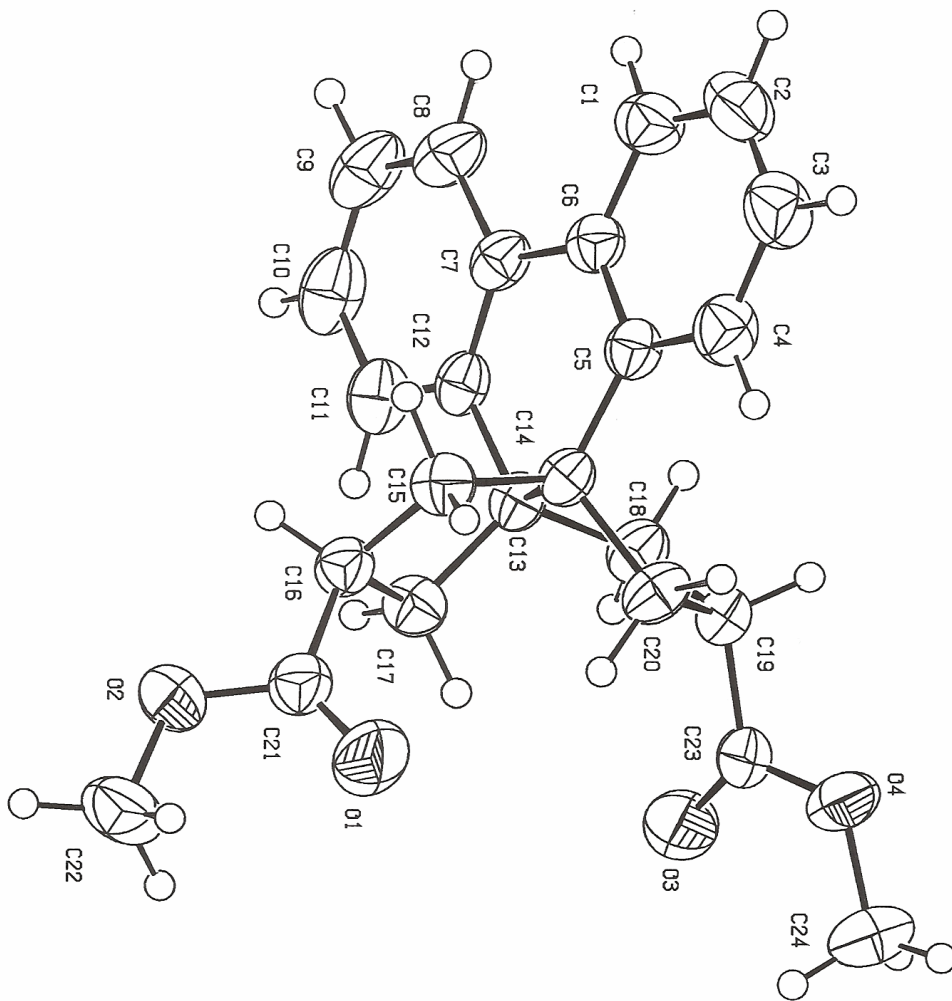


Table 10. Observed and calculated structure factors for pchm26

Page 1

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|----|---|---|------|------|-----|----|----|---|------|------|-----|----|---|---|------|------|-----|-----|----|---|------|------|-----|-----|----|---|------|------|-----|
| 3 | 0 | 0 | 173 | 174 | 1 | 6 | 9 | 0 | 75 | 72 | 1 | 1 | 3 | 1 | 342 | 363 | 3 | 10 | 7 | 1 | 13 | 11 | 4 | 0 | 13 | 1 | 46 | 51 | 1 |
| 5 | 0 | 0 | 14 | 17 | 1 | 7 | 9 | 0 | 11 | 11 | 1 | 2 | 3 | 1 | 203 | 199 | 5 | 11 | 7 | 1 | 0 | 5 | 1 | 1 | 13 | 1 | 28 | 28 | 1 |
| 6 | 0 | 0 | 212 | 209 | 1 | 8 | 9 | 0 | 0 | 5 | 1 | 3 | 3 | 1 | 570 | 552 | 5 | -12 | 8 | 1 | 12 | 2 | 9 | 2 | 13 | 1 | 31 | 34 | 1 |
| 7 | 0 | 0 | 541 | 563 | 6 | 9 | 9 | 0 | 39 | 40 | 1 | 4 | 3 | 1 | 75 | 61 | 1 | -10 | 8 | 1 | 8 | 2 | 7 | 3 | 13 | 1 | 38 | 34 | 1 |
| 8 | 0 | 0 | 221 | 225 | 2 | 0 | 10 | 0 | 133 | 131 | 1 | 5 | 3 | 1 | 59 | 66 | 1 | -9 | 8 | 1 | 108 | 94 | 1 | -5 | 14 | 1 | 0 | 7 | 1 |
| 9 | 0 | 0 | 240 | 224 | 3 | 1 | 10 | 0 | 57 | 55 | 1 | 6 | 3 | 1 | 16 | 18 | 3 | -7 | 8 | 1 | 83 | 87 | 1 | -4 | 14 | 1 | 61 | 59 | 1 |
| 10 | 0 | 0 | 0 | 14 | 1 | 2 | 10 | 0 | 81 | 76 | 1 | 7 | 3 | 1 | 147 | 144 | 1 | -6 | 8 | 1 | 73 | 76 | 1 | -3 | 14 | 1 | 12 | 10 | 2 |
| 2 | 1 | 0 | 356 | 375 | 2 | 3 | 10 | 0 | 0 | 0 | 1 | 8 | 3 | 1 | 22 | 23 | 1 | -5 | 8 | 1 | 177 | 166 | 2 | -2 | 14 | 1 | 60 | 54 | 1 |
| 3 | 1 | 0 | 111 | 108 | 1 | 4 | 10 | 0 | 119 | 147 | 1 | 9 | 3 | 1 | 32 | 31 | 1 | -4 | 8 | 1 | 1 | 6 | 1 | -1 | 14 | 1 | 84 | 74 | 1 |
| 4 | 1 | 0 | 115 | 121 | 1 | 6 | 10 | 0 | 48 | 48 | 1 | 10 | 3 | 1 | 61 | 76 | 1 | -3 | 8 | 1 | 117 | 112 | 1 | 1 | 14 | 1 | 126 | 126 | 1 |
| 5 | 1 | 0 | 342 | 331 | 6 | 7 | 10 | 0 | 15 | 12 | 1 | 11 | 3 | 1 | 17 | 16 | 4 | -2 | 8 | 1 | 108 | 102 | 1 | 3 | 14 | 1 | 11 | 24 | 4 |
| 6 | 1 | 0 | 8 | 17 | 4 | 8 | 10 | 0 | 30 | 27 | 1 | -9 | 4 | 1 | 39 | 36 | 2 | -1 | 8 | 1 | 284 | 270 | 3 | 5 | 14 | 1 | 13 | 1 | 4 |
| 7 | 1 | 0 | 239 | 233 | 2 | 9 | 10 | 0 | 9 | 12 | 2 | -7 | 4 | 1 | 67 | 60 | 1 | 1 | 8 | 1 | 47 | 52 | 1 | 6 | 14 | 1 | 47 | 44 | 1 |
| 8 | 1 | 0 | 134 | 133 | 1 | 10 | 10 | 0 | 11 | 0 | 2 | -6 | 4 | 1 | 44 | 47 | 3 | 2 | 8 | 1 | 157 | 141 | 1 | -5 | 15 | 1 | 13 | 20 | 4 |
| 9 | 1 | 0 | 11 | 6 | 4 | 1 | 11 | 0 | 48 | 50 | 1 | -5 | 4 | 1 | 57 | 56 | 1 | 3 | 8 | 1 | 58 | 53 | 1 | -4 | 15 | 1 | 43 | 40 | 1 |
| 10 | 1 | 0 | 60 | 70 | 1 | 2 | 11 | 0 | 92 | 97 | 1 | -4 | 4 | 1 | 16 | 3 | 1 | 4 | 8 | 1 | 169 | 175 | 1 | -3 | 15 | 1 | 42 | 51 | 1 |
| 1 | 2 | 0 | 216 | 219 | 2 | 3 | 11 | 0 | 243 | 239 | 3 | -3 | 4 | 1 | 454 | 450 | 4 | 5 | 8 | 1 | 45 | 46 | 1 | -1 | 15 | 1 | 0 | 10 | 1 |
| 2 | 2 | 0 | 243 | 243 | 1 | 4 | 11 | 0 | 359 | 351 | 3 | -2 | 4 | 1 | 79 | 77 | 1 | 6 | 8 | 1 | 88 | 81 | 1 | 1 | 15 | 1 | 32 | 30 | 1 |
| 3 | 2 | 0 | 134 | 138 | 2 | 5 | 11 | 0 | 39 | 41 | 1 | -1 | 4 | 1 | 169 | 175 | 1 | 7 | 8 | 1 | 234 | 230 | 2 | 2 | 15 | 1 | 0 | 14 | 1 |
| 4 | 2 | 0 | 218 | 217 | 1 | 8 | 11 | 0 | 23 | 25 | 1 | 1 | 4 | 1 | 153 | 159 | 1 | 10 | 8 | 1 | 0 | 9 | 1 | 3 | 15 | 1 | 37 | 48 | 1 |
| 5 | 2 | 0 | 11 | 18 | 4 | 10 | 11 | 0 | 52 | 42 | 1 | 2 | 4 | 1 | 330 | 330 | 2 | 11 | 8 | 1 | 33 | 46 | 2 | 4 | 15 | 1 | 23 | 30 | 2 |
| 6 | 2 | 0 | 51 | 53 | 3 | 0 | 12 | 0 | 177 | 175 | 2 | 3 | 4 | 1 | 74 | 77 | 1 | -11 | 9 | 1 | 15 | 12 | 2 | 5 | 15 | 1 | 8 | 16 | 8 |
| 7 | 2 | 0 | 181 | 188 | 1 | 1 | 12 | 0 | 39 | 41 | 1 | 4 | 4 | 1 | 141 | 129 | 1 | -9 | 9 | 1 | 14 | 9 | 2 | -4 | 16 | 1 | 54 | 48 | 1 |
| 8 | 2 | 0 | 113 | 112 | 1 | 2 | 12 | 0 | 48 | 54 | 1 | 5 | 4 | 1 | 103 | 107 | 1 | -8 | 9 | 1 | 71 | 63 | 1 | -3 | 16 | 1 | 0 | 8 | 1 |
| 9 | 2 | 0 | 30 | 27 | 5 | 4 | 12 | 0 | 54 | 54 | 1 | 6 | 4 | 1 | 235 | 236 | 4 | -7 | 9 | 1 | 50 | 49 | 1 | 1 | 16 | 1 | 21 | 25 | 1 |
| 10 | 2 | 0 | 40 | 49 | 1 | 5 | 12 | 0 | 26 | 28 | 1 | 7 | 4 | 1 | 81 | 81 | 1 | -6 | 9 | 1 | 14 | 14 | 1 | 2 | 16 | 1 | 26 | 27 | 1 |
| 2 | 3 | 0 | 219 | 220 | 2 | 6 | 12 | 0 | 60 | 61 | 1 | 8 | 4 | 1 | 50 | 50 | 1 | -5 | 9 | 1 | 58 | 68 | 1 | 4 | 16 | 1 | 15 | 11 | 4 |
| 3 | 3 | 0 | 278 | 268 | 3 | 2 | 13 | 0 | 63 | 58 | 1 | -9 | 4 | 1 | 12 | 14 | 3 | -4 | 9 | 1 | 98 | 68 | 1 | 5 | 16 | 1 | 43 | 38 | 1 |
| 4 | 3 | 0 | 347 | 339 | 3 | 3 | 13 | 0 | 109 | 106 | 1 | -8 | 5 | 1 | 22 | 33 | 2 | -2 | 9 | 1 | 6 | 10 | 6 | 5 | 16 | 1 | 43 | 38 | 1 |
| 5 | 3 | 0 | 191 | 194 | 2 | 4 | 13 | 0 | 20 | 23 | 1 | -8 | 5 | 1 | 122 | 114 | 1 | -1 | 9 | 1 | 60 | 63 | 1 | 2 | 17 | 1 | 12 | 8 | 1 |
| 6 | 3 | 0 | 18 | 15 | 1 | 5 | 13 | 0 | 18 | 19 | 2 | -7 | 5 | 1 | 137 | 144 | 1 | 0 | 9 | 1 | 186 | 177 | 1 | 4 | 17 | 1 | 96 | 84 | 1 |
| 7 | 3 | 0 | 153 | 154 | 1 | 6 | 13 | 0 | 18 | 19 | 2 | -6 | 5 | 1 | 147 | 141 | 1 | 1 | 9 | 1 | 113 | 112 | 1 | 5 | 17 | 1 | 25 | 30 | 2 |
| 8 | 3 | 0 | 27 | 34 | 1 | 1 | 14 | 0 | 28 | 28 | 1 | -5 | 5 | 1 | 146 | 144 | 1 | 3 | 9 | 1 | 119 | 122 | 1 | -5 | 18 | 1 | 13 | 1 | 6 |
| 9 | 3 | 0 | 35 | 29 | 1 | 2 | 14 | 0 | 0 | 8 | 1 | -4 | 5 | 1 | 253 | 239 | 1 | 4 | 9 | 1 | 104 | 105 | 1 | -4 | 18 | 1 | 11 | 9 | 4 |
| 10 | 3 | 0 | 14 | 18 | 4 | 3 | 14 | 0 | 24 | 27 | 1 | -3 | 5 | 1 | 213 | 215 | 1 | 5 | 9 | 1 | 87 | 85 | 1 | -3 | 18 | 1 | 35 | 48 | 1 |
| 1 | 4 | 0 | 291 | 298 | 2 | 4 | 14 | 0 | 11 | 1 | 3 | -2 | 5 | 1 | 492 | 485 | 4 | 6 | 9 | 1 | 0 | 5 | 1 | 2 | 18 | 1 | 14 | 11 | 1 |
| 2 | 4 | 0 | 50 | 50 | 1 | 1 | 15 | 0 | 92 | 83 | 1 | -1 | 5 | 1 | 27 | 36 | 1 | 7 | 9 | 1 | 84 | 86 | 1 | 3 | 18 | 1 | 12 | 8 | 3 |
| 3 | 4 | 0 | 65 | 76 | 1 | 2 | 15 | 0 | 61 | 51 | 1 | 0 | 5 | 1 | 43 | 42 | 1 | 9 | 9 | 1 | 0 | 13 | 1 | 5 | 18 | 1 | 25 | 22 | 3 |
| 4 | 4 | 0 | 34 | 34 | 1 | 3 | 15 | 0 | 0 | 7 | 1 | 1 | 5 | 1 | 349 | 343 | 4 | 11 | 9 | 1 | 21 | 21 | 2 | -3 | 19 | 1 | 18 | 22 | 1 |
| 5 | 4 | 0 | 8 | 5 | 2 | 1 | 16 | 0 | 9 | 6 | 1 | 2 | 5 | 1 | 113 | 107 | 1 | -11 | 10 | 1 | 74 | 65 | 1 | 3 | 19 | 1 | 21 | 24 | 1 |
| 6 | 4 | 0 | 53 | 56 | 4 | 2 | 16 | 0 | 37 | 29 | 1 | 3 | 5 | 1 | 206 | 208 | 1 | -8 | 10 | 1 | 44 | 41 | 1 | -10 | 0 | 2 | 17 | 18 | 3 |
| 7 | 4 | 0 | 21 | 19 | 1 | 3 | 16 | 0 | 9 | 5 | 5 | 4 | 5 | 1 | 39 | 34 | 1 | -7 | 10 | 1 | 83 | 80 | 1 | -8 | 0 | 2 | 79 | 77 | 1 |
| 8 | 4 | 0 | 70 | 73 | 1 | 2 | 17 | 0 | 33 | 30 | 1 | 5 | 5 | 1 | 220 | 215 | 1 | -6 | 10 | 1 | 28 | 30 | 1 | -7 | 0 | 2 | 329 | 329 | 4 |
| 9 | 4 | 0 | 10 | 22 | 5 | 5 | 17 | 0 | 0 | 5 | 1 | 6 | 5 | 1 | 78 | 74 | 1 | -5 | 10 | 1 | 151 | 146 | 1 | -6 | 0 | 2 | 0 | 1 | 1 |
| 10 | 4 | 0 | 11 | 7 | 5 | 3 | 18 | 0 | 10 | 10 | 4 | 7 | 5 | 1 | 124 | 119 | 3 | -3 | 10 | 1 | 90 | 84 | 1 | -5 | 0 | 2 | 242 | 227 | 2 |
| 11 | 4 | 0 | 0 | 11 | 1 | 3 | 19 | 0 | 16 | 16 | 1 | 8 | 5 | 1 | 59 | 60 | 1 | -2 | 10 | 1 | 74 | 79 | 1 | -4 | 0 | 2 | 157 | 170 | 1 |
| 1 | 5 | 0 | 25 | 27 | 1 | 4 | 19 | 0 | 0 | 5 | 1 | 9 | 5 | 1 | 39 | 35 | 1 | -1 | 10 | 1 | 55 | 49 | 1 | -3 | 0 | 2 | 333 | 341 | 2 |
| 2 | 5 | 0 | 107 | 117 | 2 | -9 | 1 | 1 | 13 | 7 | 3 | 10 | 5 | 1 | 43 | 37 | 1 | 0 | 10 | 1 | 72 | 77 | 1 | -1 | 0 | 2 | 319 | 381 | 4 |
| 3 | 5 | 0 | 30 | 35 | 1 | -7 | 1 | 1 | 246 | 248 | 2 | 11 | 5 | 1 | 38 | 32 | 1 | 1 | 10 | 1 | 85 | 86 | 1 | 3 | 0 | 2 | 193 | 183 | 1 |
| 4 | 5 | 0 | 12 | 6 | 2 | -6 | 1 | 1 | 66 | 62 | 1 | -9 | 6 | 1 | 9 | 17 | 6 | 2 | 10 | 1 | 61 | 56 | 1 | 4 | 0 | 2 | 329 | 311 | 2 |
| 5 | 5 | 0 | 88 | 92 | 1 | -5 | 1 | 1 | 5 | 5 | 5 | -8 | 6 | 1 | 16 | 25 | 2 | 4 | 10 | 1 | 60 | 60 | 1 | 5 | 0 | 2 | 16 | 24 | 1 |
| 6 | 5 | 0 | 189 | 189 | 1 | -4 | 1 | 1 | 192 | 199 | 1 | -7 | 6 | 1 | 295 | 309 | 8 | 5 | 10 | 1 | 12 | 12 | 2 | 7 | 0 | 2 | 165 | 182 | 2 |
| 7 | 5 | 0 | 11 | 14 | 2 | -3 | 1 | 1 | 315 | 324 | 1 | -6 | 6 | 1 | 0 | 4 | 1 | 6 | 10 | 1 | 73 | 73 | 1 | 8 | 0 | 2 | 80 | 100 | 1 |
| 9 | 5 | 0 | 66 | 61 | 3 | -2 | 1 | 1 | 127 | 129 | 2 | -5 | 6 | 1 | 156 | 154 | 1 | 8 | 10 | 1 | 9 | 7 | 2 | 9 | 0 | 2 | 12 | 2 | 6 |
| 10 | 5 | 0 | 33 | 37 | 1 | 1 | 1 | 1 | 160 | 163 | 1 | -4 | 6 | 1 | 147 | 145 | 1 | 9 | 10 | 1 | 14 | 21 | 2 | -11 | 1 | 2 | 34 | 30 | 2 |
| 0 | 6 | 0 | 332 | 300 | 4 | 2 | 1 | 1 | 31 | 27 | 1 | -3 | 6 | 1 | 24 | 28 | 1 | 11 | 10 | 1 | 12 | 1 | 5 | -8 | 1 | 2 | 10 | 12 | 7 |
| 1 | 6 | 0 | 393 | 390 | 3 | 3 | 1 | 1 | 144 | 140 | 1 | -2 | 6 | 1 | 48 | 48 | 1 | -11 | 11 | 1 | 22 | 21 | 1 | -7 | 1 | 2 | 117 | 121 | 1 |
| 2 | 6 | 0 | 47 | 50 | 1 | 4 | 1 | 1 | 212 | 206 | 2 | -1 | 6 | 1 | 152 | 160 | 1 | -8 | 11 | 1 | 9 | 7 | 1 | -6 | 1 | 2 | 108 | 102 | 1 |
| 3 | 6 | 0 | 122 | 127 | 1 | 5 | 1 | 1 | 96 | 97 | 1 | 0 | 6 | 1 | 440 | 447 | 5 | -6 | 11 | 1 | 23 | 34 | 2 | -5 | 1 | 2 | 127 | 131 | 1 |
| 4 | 6 | 0 | 191 | 184 | 1 | 6 | 1 | 1 | 50 | 45 | 1 | 1 | 6 | 1 | 95 | 98 | 1 | -5 | 11 | 1 | 42 | 40 | 1 | -4 | 1 | 2 | 132 | 144 | 1 |
| 5 | 6 | 0 | 214 | 220 | | | | | | | | | | | | | | | | | | | | | | | | | |

Table 10. Observed and calculated structure factors for pchm26

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | | | | | | |
|-----|---|---|------|------|-----|-----|----|---|------|------|-----|----|----|---|------|------|-----|-----|---|---|------|------|-----|-----|----|---|-----|-----|---|
| 7 | 2 | 2 | 139 | 138 | 1 | -4 | 7 | 2 | 98 | 87 | 1 | -3 | 12 | 2 | 48 | 47 | 1 | 8 | 2 | 3 | 102 | 103 | 8 | 0 | 7 | 3 | 227 | 223 | 1 |
| 8 | 2 | 2 | 32 | 32 | 1 | -3 | 7 | 2 | 76 | 63 | 1 | -1 | 12 | 2 | 118 | 124 | 1 | 9 | 2 | 3 | 18 | 18 | 3 | 1 | 7 | 3 | 136 | 137 | 2 |
| 9 | 2 | 2 | 29 | 29 | 2 | -2 | 7 | 2 | 161 | 157 | 1 | 0 | 12 | 2 | 142 | 136 | 2 | -11 | 3 | 3 | 15 | 6 | 4 | 2 | 7 | 3 | 152 | 153 | 1 |
| -11 | 3 | 2 | 12 | 25 | 0 | -1 | 7 | 2 | 422 | 383 | 3 | 1 | 12 | 2 | 58 | 55 | 1 | -10 | 3 | 3 | 13 | 14 | 10 | 3 | 7 | 3 | 276 | 268 | 2 |
| -9 | 3 | 2 | 42 | 43 | 1 | 0 | 7 | 2 | 306 | 274 | 2 | 3 | 12 | 2 | 61 | 58 | 1 | -9 | 3 | 3 | 11 | 10 | 5 | 4 | 7 | 3 | 27 | 30 | 1 |
| -8 | 3 | 2 | 86 | 81 | 1 | 1 | 7 | 2 | 262 | 248 | 2 | 5 | 12 | 2 | 48 | 48 | 1 | -8 | 3 | 3 | 7 | 3 | 6 | 5 | 7 | 3 | 131 | 127 | 1 |
| -7 | 3 | 2 | 9 | 15 | 5 | 2 | 7 | 2 | 84 | 83 | 1 | -7 | 13 | 2 | 17 | 18 | 4 | -7 | 3 | 3 | 67 | 68 | 1 | 6 | 7 | 3 | 33 | 38 | 3 |
| -6 | 3 | 2 | 12 | 13 | 1 | 3 | 7 | 2 | 196 | 179 | 3 | -5 | 13 | 2 | 25 | 29 | 1 | -6 | 3 | 3 | 224 | 218 | 2 | 7 | 7 | 3 | 39 | 45 | 1 |
| -5 | 3 | 2 | 128 | 123 | 2 | 4 | 7 | 2 | 19 | 14 | 9 | -4 | 13 | 2 | 88 | 82 | 1 | -5 | 3 | 3 | 60 | 57 | 1 | 8 | 7 | 3 | 11 | 4 | 2 |
| -3 | 3 | 2 | 258 | 271 | 2 | 5 | 7 | 2 | 166 | 172 | 1 | -1 | 13 | 2 | 0 | 1 | 1 | -4 | 3 | 3 | 80 | 85 | 1 | 9 | 7 | 3 | 54 | 53 | 1 |
| -1 | 3 | 2 | 108 | 110 | 1 | 6 | 7 | 2 | 62 | 64 | 1 | 0 | 13 | 2 | 14 | 13 | 1 | -3 | 3 | 3 | 8 | 8 | 1 | 10 | 7 | 3 | 46 | 40 | 1 |
| 0 | 3 | 2 | 345 | 348 | 2 | 8 | 7 | 2 | 21 | 26 | 1 | 1 | 13 | 2 | 10 | 12 | 1 | -2 | 3 | 3 | 441 | 445 | 3 | -11 | 8 | 3 | 0 | 4 | 1 |
| 1 | 3 | 2 | 195 | 206 | 2 | -12 | 8 | 2 | 30 | 24 | 2 | 2 | 13 | 2 | 19 | 13 | 1 | 0 | 3 | 3 | 149 | 161 | 1 | -10 | 8 | 3 | 0 | 12 | 1 |
| 2 | 3 | 2 | 180 | 184 | 1 | -11 | 8 | 2 | 16 | 17 | 3 | 3 | 13 | 2 | 122 | 118 | 1 | 1 | 3 | 3 | 457 | 459 | 4 | -9 | 8 | 3 | 7 | 20 | 7 |
| 3 | 3 | 2 | 174 | 167 | 1 | -10 | 8 | 2 | 14 | 10 | 3 | 4 | 13 | 2 | 53 | 53 | 1 | 2 | 3 | 3 | 113 | 118 | 1 | -8 | 8 | 3 | 107 | 98 | 1 |
| 4 | 3 | 2 | 134 | 123 | 1 | -9 | 8 | 2 | 18 | 28 | 1 | -5 | 14 | 2 | 83 | 79 | 1 | 3 | 3 | 3 | 182 | 172 | 1 | -7 | 8 | 3 | 6 | 6 | 6 |
| 5 | 3 | 2 | 70 | 59 | 1 | -8 | 8 | 2 | 9 | 12 | 3 | -4 | 14 | 2 | 72 | 73 | 1 | 4 | 3 | 3 | 29 | 20 | 1 | -6 | 8 | 3 | 78 | 83 | 1 |
| 6 | 3 | 2 | 82 | 82 | 1 | -7 | 8 | 2 | 10 | 11 | 1 | -2 | 14 | 2 | 9 | 5 | 4 | 5 | 3 | 3 | 104 | 108 | 1 | -5 | 8 | 3 | 18 | 26 | 3 |
| 7 | 3 | 2 | 0 | 10 | 1 | -6 | 8 | 2 | 80 | 84 | 1 | -1 | 14 | 2 | 126 | 125 | 1 | 7 | 3 | 3 | 222 | 219 | 2 | -4 | 8 | 3 | 131 | 128 | 3 |
| 8 | 3 | 2 | 13 | 11 | 2 | -5 | 8 | 2 | 42 | 45 | 2 | 1 | 14 | 2 | 11 | 10 | 1 | 8 | 3 | 3 | 13 | 19 | 5 | -3 | 8 | 3 | 113 | 103 | 3 |
| 9 | 3 | 2 | 74 | 67 | 1 | -4 | 8 | 2 | 67 | 79 | 1 | 3 | 14 | 2 | 37 | 43 | 1 | 9 | 3 | 3 | 17 | 26 | 3 | -2 | 8 | 3 | 67 | 62 | 1 |
| 10 | 3 | 2 | 25 | 28 | 2 | -3 | 8 | 2 | 59 | 59 | 1 | 4 | 14 | 2 | 29 | 30 | 1 | -9 | 4 | 3 | 20 | 28 | 1 | -1 | 8 | 3 | 101 | 86 | 1 |
| -10 | 4 | 2 | 10 | 5 | 4 | -2 | 8 | 2 | 185 | 191 | 1 | 5 | 14 | 2 | 0 | 3 | 1 | -8 | 4 | 3 | 54 | 54 | 1 | 0 | 8 | 3 | 205 | 199 | 1 |
| -9 | 4 | 2 | 0 | 3 | 1 | -1 | 8 | 2 | 56 | 52 | 1 | -6 | 15 | 2 | 34 | 37 | 1 | -7 | 4 | 3 | 0 | 2 | 1 | 1 | 8 | 3 | 76 | 86 | 1 |
| -8 | 4 | 2 | 66 | 66 | 5 | 0 | 8 | 2 | 207 | 200 | 3 | -5 | 15 | 2 | 20 | 21 | 2 | -6 | 4 | 3 | 156 | 157 | 1 | 2 | 8 | 3 | 23 | 22 | 1 |
| -7 | 4 | 2 | 200 | 199 | 5 | 1 | 8 | 2 | 188 | 197 | 6 | -4 | 15 | 2 | 58 | 45 | 1 | -5 | 4 | 3 | 78 | 79 | 1 | 3 | 8 | 3 | 240 | 238 | 1 |
| -6 | 4 | 2 | 143 | 140 | 1 | 2 | 8 | 2 | 76 | 72 | 1 | -3 | 15 | 2 | 40 | 49 | 1 | -4 | 4 | 3 | 258 | 241 | 3 | 4 | 8 | 3 | 142 | 145 | 1 |
| -5 | 4 | 2 | 8 | 16 | 3 | 3 | 8 | 2 | 7 | 12 | 1 | -2 | 15 | 2 | 72 | 64 | 1 | -3 | 4 | 3 | 167 | 160 | 1 | 5 | 8 | 3 | 67 | 66 | 1 |
| -4 | 4 | 2 | 506 | 485 | 3 | 4 | 8 | 2 | 127 | 128 | 1 | -1 | 15 | 2 | 27 | 31 | 1 | -2 | 4 | 3 | 19 | 11 | 1 | 6 | 8 | 3 | 80 | 78 | 1 |
| -3 | 4 | 2 | 173 | 184 | 1 | 5 | 8 | 2 | 72 | 71 | 1 | 1 | 15 | 2 | 0 | 1 | 1 | -1 | 4 | 3 | 296 | 290 | 2 | 7 | 8 | 3 | 31 | 36 | 1 |
| -2 | 4 | 2 | 261 | 257 | 1 | 6 | 8 | 2 | 95 | 106 | 1 | 3 | 15 | 2 | 20 | 18 | 1 | 0 | 4 | 3 | 203 | 199 | 2 | 8 | 8 | 3 | 26 | 30 | 1 |
| -1 | 4 | 2 | 59 | 56 | 1 | 7 | 8 | 2 | 22 | 18 | 1 | 4 | 15 | 2 | 101 | 91 | 1 | 1 | 4 | 3 | 170 | 165 | 2 | -12 | 9 | 3 | 19 | 14 | 3 |
| 0 | 4 | 2 | 240 | 231 | 4 | 8 | 8 | 2 | 36 | 38 | 1 | -6 | 16 | 2 | 14 | 10 | 5 | 2 | 4 | 3 | 98 | 100 | 1 | -11 | 9 | 3 | 12 | 9 | 5 |
| 1 | 4 | 2 | 10 | 13 | 2 | 9 | 8 | 2 | 10 | 4 | 3 | -3 | 16 | 2 | 0 | 2 | 1 | 3 | 4 | 3 | 366 | 346 | 2 | -10 | 9 | 3 | 2 | 5 | 2 |
| 2 | 4 | 2 | 552 | 530 | 4 | -10 | 9 | 2 | 7 | 6 | 7 | -2 | 16 | 2 | 46 | 47 | 1 | 4 | 4 | 3 | 142 | 144 | 1 | -9 | 9 | 3 | 53 | 45 | 1 |
| 3 | 4 | 2 | 494 | 487 | 5 | -9 | 9 | 2 | 0 | 8 | 1 | 1 | 16 | 2 | 32 | 31 | 1 | 5 | 4 | 3 | 151 | 146 | 1 | -8 | 9 | 3 | 13 | 14 | 1 |
| 4 | 4 | 2 | 153 | 147 | 1 | -8 | 9 | 2 | 50 | 48 | 1 | 3 | 16 | 2 | 41 | 33 | 1 | 6 | 4 | 3 | 28 | 29 | 1 | -7 | 9 | 3 | 36 | 31 | 2 |
| 5 | 4 | 2 | 55 | 53 | 1 | -7 | 9 | 2 | 144 | 148 | 1 | 4 | 16 | 2 | 13 | 13 | 5 | 7 | 4 | 3 | 120 | 131 | 1 | -6 | 9 | 3 | 14 | 21 | 1 |
| 6 | 4 | 2 | 158 | 155 | 1 | -5 | 9 | 2 | 14 | 16 | 1 | -6 | 17 | 2 | 0 | 9 | 1 | 8 | 4 | 3 | 0 | 3 | 1 | -5 | 9 | 3 | 12 | 10 | 1 |
| 7 | 4 | 2 | 87 | 100 | 3 | -4 | 9 | 2 | 159 | 154 | 2 | -4 | 17 | 2 | 14 | 13 | 4 | -12 | 5 | 3 | 7 | 1 | 7 | -4 | 9 | 3 | 142 | 143 | 1 |
| 8 | 4 | 2 | 86 | 84 | 1 | -3 | 9 | 2 | 99 | 92 | 1 | -3 | 17 | 2 | 36 | 34 | 1 | -10 | 5 | 3 | 22 | 18 | 2 | -3 | 9 | 3 | 172 | 170 | 1 |
| -12 | 5 | 2 | 16 | 9 | 5 | -1 | 9 | 2 | 12 | 6 | 1 | -2 | 17 | 2 | 44 | 44 | 1 | -8 | 5 | 3 | 86 | 90 | 1 | -2 | 9 | 3 | 16 | 13 | 1 |
| -11 | 5 | 2 | 28 | 28 | 2 | 0 | 9 | 2 | 68 | 66 | 1 | 1 | 17 | 2 | 11 | 12 | 1 | -7 | 5 | 3 | 148 | 150 | 2 | -1 | 9 | 3 | 45 | 36 | 2 |
| -10 | 5 | 2 | 13 | 11 | 4 | 1 | 9 | 2 | 133 | 135 | 1 | 2 | 17 | 2 | 9 | 5 | 3 | -6 | 5 | 3 | 124 | 127 | 1 | 0 | 9 | 3 | 139 | 147 | 1 |
| -9 | 5 | 2 | 61 | 58 | 1 | 2 | 9 | 2 | 98 | 94 | 1 | 3 | 17 | 2 | 16 | 11 | 2 | -5 | 5 | 3 | 0 | 4 | 1 | 1 | 9 | 3 | 157 | 160 | 3 |
| -8 | 5 | 2 | 186 | 189 | 2 | 3 | 9 | 2 | 81 | 83 | 1 | -6 | 18 | 2 | 0 | 3 | 1 | -4 | 5 | 3 | 311 | 309 | 3 | 2 | 9 | 3 | 161 | 153 | 1 |
| -7 | 5 | 2 | 0 | 2 | 1 | 4 | 9 | 2 | 123 | 131 | 1 | -5 | 18 | 2 | 10 | 10 | 8 | -3 | 5 | 3 | 88 | 80 | 1 | 3 | 9 | 3 | 344 | 340 | 3 |
| -6 | 5 | 2 | 148 | 157 | 1 | 5 | 9 | 2 | 117 | 118 | 3 | -4 | 18 | 2 | 31 | 46 | 1 | -1 | 5 | 3 | 132 | 125 | 2 | 4 | 9 | 3 | 236 | 237 | 1 |
| -5 | 5 | 2 | 202 | 187 | 1 | 7 | 9 | 2 | 6 | 4 | 4 | -3 | 18 | 2 | 37 | 40 | 1 | 0 | 5 | 3 | 115 | 107 | 1 | 5 | 9 | 3 | 9 | 2 | 1 |
| -4 | 5 | 2 | 184 | 183 | 1 | 8 | 9 | 2 | 24 | 25 | 1 | 2 | 18 | 2 | 43 | 41 | 1 | 1 | 5 | 3 | 275 | 276 | 2 | 6 | 9 | 3 | 74 | 70 | 1 |
| -3 | 5 | 2 | 106 | 106 | 2 | 9 | 9 | 2 | 0 | 7 | 1 | 3 | 18 | 2 | 50 | 47 | 1 | 2 | 5 | 3 | 142 | 134 | 1 | 7 | 9 | 3 | 50 | 47 | 1 |
| -1 | 5 | 2 | 164 | 163 | 1 | 10 | 9 | 2 | 11 | 1 | 6 | -3 | 19 | 2 | 7 | 4 | 5 | 3 | 5 | 3 | 278 | 275 | 1 | 8 | 9 | 3 | 9 | 25 | 4 |
| 1 | 5 | 2 | 141 | 151 | 1 | -11 | 10 | 2 | 0 | 19 | 1 | 3 | 19 | 2 | 19 | 27 | 2 | 4 | 5 | 3 | 203 | 193 | 1 | 9 | 9 | 3 | 54 | 48 | 1 |
| 2 | 5 | 2 | 183 | 169 | 1 | -10 | 10 | 2 | 11 | 10 | 1 | 4 | 19 | 2 | 0 | 1 | 1 | 5 | 5 | 3 | 211 | 208 | 1 | 10 | 9 | 3 | 62 | 53 | 1 |
| 3 | 5 | 2 | 197 | 191 | 1 | -8 | 10 | 2 | 28 | 25 | 1 | -9 | 1 | 3 | 83 | 83 | 1 | 6 | 5 | 3 | 6 | 16 | 5 | -10 | 10 | 3 | 9 | 1 | 4 |
| 4 | 5 | 2 | 108 | 109 | 1 | -7 | 10 | 2 | 29 | 28 | 1 | -8 | 1 | 3 | 436 | 435 | 8 | 9 | 5 | 3 | 11 | 19 | 5 | -8 | 10 | 3 | 54 | 48 | 1 |
| 5 | 5 | 2 | 75 | 78 | 1 | -6 | 10 | 2 | 10 | 15 | 7 | -7 | 1 | 3 | 396 | 404 | 2 | 10 | 5 | 3 | 0 | 6 | 1 | -7 | 10 | 3 | 7 | 13 | 2 |
| 6 | 5 | 2 | 111 | 107 | 1 | -4 | 10 | 2 | 48 | 51 | 1 | -6 | 1 | 3 | 114 | 104 | 1 | -10 | 6 | 3 | 0 | 4 | 1 | -6 | 10 | 3 | 22 | 20 | 1 |
| 7 | 5 | 2 | 208 | 234 | 2 | -3 | 10 | 2 | 9 | 11 | 3 | -5 | 1 | 3 | 51 | 44 | 1 | -8 | 6 | 3 | 0 | 1 | 1 | -4 | 10 | 3 | 499 | 481 | 4 |
| 8 | 5 | 2 | 0 | 9 | 1 | -2 | 10 | 2 | 35 | 34 | 1 | -4 | 1 | 3 | 24 | 24 | 1 | -7 | 6 | 3 | 74 | 80 | 3 | -3 | 10 | 3 | 214 | 209 | 1 |
| 9 | 5 | 2 | 8 | 6 | 8 | -1 | 10 | 2 | 6 | 2 | 2 | -3 | | | | | | | | | | | | | | | | | |

Table 10. Observed and calculated structure factors for pchm26

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|----|----|---|------|------|-----|-----|---|---|------|------|-----|-----|---|---|------|------|-----|-----|----|---|------|------|-----|-----|---|---|------|------|-----|
| 5 | 11 | 3 | 0 | 15 | 1 | 4 | 1 | 4 | 307 | 299 | 2 | -4 | 6 | 4 | 137 | 130 | 2 | 2 | 10 | 4 | 68 | 74 | 1 | -6 | 1 | 5 | 71 | 77 | 1 |
| 7 | 11 | 3 | 0 | 8 | 1 | 5 | 1 | 4 | 69 | 72 | 1 | -3 | 6 | 4 | 241 | 249 | 3 | 3 | 10 | 4 | 8 | 8 | 1 | -5 | 1 | 5 | 43 | 43 | 1 |
| 9 | 11 | 3 | 17 | 16 | 1 | 6 | 1 | 4 | 105 | 108 | 1 | -2 | 6 | 4 | 247 | 246 | 1 | 4 | 10 | 4 | 86 | 85 | 1 | -4 | 1 | 5 | 208 | 210 | 1 |
| 10 | 11 | 3 | 10 | 1 | 7 | 7 | 1 | 4 | 59 | 69 | 1 | -1 | 6 | 4 | 259 | 267 | 2 | 5 | 10 | 4 | 65 | 63 | 1 | -3 | 1 | 5 | 62 | 70 | 2 |
| -6 | 12 | 3 | 66 | 69 | 1 | 8 | 1 | 4 | 67 | 62 | 1 | 0 | 6 | 4 | 195 | 188 | 1 | 6 | 10 | 4 | 39 | 41 | 1 | -1 | 1 | 5 | 364 | 354 | 2 |
| -4 | 12 | 3 | 257 | 248 | 2 | -10 | 2 | 4 | 5 | 1 | 5 | 1 | 6 | 4 | 195 | 199 | 1 | 7 | 10 | 4 | 26 | 36 | 2 | 0 | 1 | 5 | 191 | 193 | 2 |
| -3 | 12 | 3 | 55 | 63 | 1 | -9 | 2 | 4 | 14 | 22 | 3 | 2 | 6 | 4 | 114 | 122 | 1 | 8 | 10 | 4 | 0 | 0 | 1 | 1 | 1 | 5 | 469 | 458 | 2 |
| -2 | 12 | 3 | 53 | 54 | 1 | -8 | 2 | 4 | 36 | 37 | 2 | 3 | 6 | 4 | 30 | 37 | 1 | -11 | 11 | 4 | 64 | 57 | 1 | 2 | 1 | 5 | 6 | 4 | 2 |
| -1 | 12 | 3 | 80 | 84 | 1 | -7 | 2 | 4 | 96 | 100 | 1 | 4 | 6 | 4 | 48 | 47 | 1 | -10 | 11 | 4 | 0 | 4 | 1 | 3 | 1 | 5 | 311 | 308 | 1 |
| 0 | 12 | 3 | 228 | 220 | 4 | -6 | 2 | 4 | 82 | 79 | 1 | 5 | 6 | 4 | 281 | 272 | 2 | -9 | 11 | 4 | 45 | 43 | 1 | 4 | 1 | 5 | 116 | 109 | 1 |
| 1 | 12 | 3 | 154 | 148 | 1 | -5 | 2 | 4 | 46 | 51 | 1 | 6 | 6 | 4 | 83 | 85 | 1 | -8 | 11 | 4 | 30 | 29 | 1 | 5 | 1 | 5 | 6 | 1 | 6 |
| 2 | 12 | 3 | 12 | 14 | 2 | -4 | 2 | 4 | 500 | 495 | 5 | 7 | 6 | 4 | 153 | 165 | 9 | -6 | 11 | 4 | 21 | 18 | 1 | 6 | 1 | 5 | 121 | 122 | 1 |
| 3 | 12 | 3 | 87 | 108 | 1 | -3 | 2 | 4 | 83 | 79 | 1 | 8 | 6 | 4 | 43 | 43 | 1 | -5 | 11 | 4 | 137 | 135 | 1 | 7 | 1 | 5 | 90 | 89 | 1 |
| 5 | 12 | 3 | 41 | 45 | 1 | -2 | 2 | 4 | 84 | 81 | 2 | 9 | 6 | 4 | 46 | 39 | 1 | -4 | 11 | 4 | 29 | 25 | 1 | -10 | 2 | 5 | 0 | 3 | 1 |
| 6 | 12 | 3 | 19 | 14 | 3 | -1 | 2 | 4 | 475 | 483 | 7 | 10 | 6 | 4 | 26 | 30 | 2 | -2 | 11 | 4 | 60 | 62 | 1 | -9 | 2 | 5 | 21 | 22 | 2 |
| -6 | 13 | 3 | 23 | 23 | 2 | 0 | 2 | 4 | 506 | 500 | 6 | -12 | 7 | 4 | 0 | 4 | 1 | -1 | 11 | 4 | 20 | 20 | 2 | -8 | 2 | 5 | 129 | 128 | 1 |
| -4 | 13 | 3 | 102 | 94 | 1 | 1 | 2 | 4 | 239 | 245 | 1 | -11 | 7 | 4 | 14 | 2 | 4 | 0 | 11 | 4 | 193 | 196 | 1 | -7 | 2 | 5 | 76 | 78 | 1 |
| -3 | 13 | 3 | 40 | 44 | 1 | 2 | 2 | 4 | 160 | 163 | 2 | -9 | 7 | 4 | 38 | 36 | 1 | 1 | 11 | 4 | 65 | 66 | 1 | -6 | 2 | 5 | 107 | 112 | 1 |
| -2 | 13 | 3 | 12 | 13 | 1 | 3 | 2 | 4 | 627 | 591 | 4 | -8 | 7 | 4 | 178 | 191 | 2 | 2 | 11 | 4 | 9 | 5 | 3 | -5 | 2 | 5 | 263 | 259 | 1 |
| -1 | 13 | 3 | 21 | 25 | 9 | 4 | 2 | 4 | 101 | 102 | 1 | -7 | 7 | 4 | 107 | 115 | 1 | -7 | 11 | 4 | 74 | 71 | 1 | -4 | 2 | 5 | 60 | 61 | 1 |
| 0 | 13 | 3 | 65 | 69 | 3 | 5 | 2 | 4 | 232 | 225 | 2 | -6 | 7 | 4 | 106 | 114 | 1 | 5 | 11 | 4 | 10 | 11 | 1 | -3 | 2 | 5 | 18 | 12 | 5 |
| 5 | 13 | 3 | 14 | 10 | 3 | 6 | 2 | 4 | 12 | 15 | 2 | -5 | 7 | 4 | 132 | 119 | 1 | 7 | 11 | 4 | 90 | 81 | 1 | -2 | 2 | 5 | 163 | 170 | 2 |
| -7 | 14 | 3 | 18 | 21 | 3 | 7 | 2 | 4 | 144 | 136 | 1 | -4 | 7 | 4 | 169 | 172 | 1 | 8 | 11 | 4 | 14 | 9 | 1 | -1 | 2 | 5 | 480 | 479 | 3 |
| -6 | 14 | 3 | 15 | 11 | 5 | 8 | 2 | 4 | 29 | 31 | 1 | -3 | 7 | 4 | 198 | 192 | 1 | 9 | 11 | 4 | 15 | 12 | 2 | 0 | 2 | 5 | 336 | 339 | 2 |
| -3 | 14 | 3 | 102 | 94 | 1 | -11 | 3 | 4 | 20 | 20 | 3 | -2 | 7 | 4 | 72 | 75 | 1 | -7 | 12 | 4 | 49 | 45 | 1 | 1 | 2 | 5 | 445 | 442 | 2 |
| -2 | 14 | 3 | 17 | 13 | 1 | -9 | 3 | 4 | 12 | 15 | 4 | -1 | 7 | 4 | 70 | 71 | 1 | -3 | 12 | 4 | 22 | 23 | 1 | 3 | 2 | 5 | 300 | 296 | 1 |
| -1 | 14 | 3 | 94 | 82 | 1 | -8 | 3 | 4 | 102 | 111 | 11 | 0 | 7 | 4 | 7 | 7 | 1 | -2 | 12 | 4 | 46 | 51 | 1 | 4 | 2 | 5 | 89 | 91 | 1 |
| 0 | 14 | 3 | 14 | 8 | 1 | -7 | 3 | 4 | 202 | 215 | 14 | 2 | 7 | 4 | 90 | 83 | 1 | 0 | 12 | 4 | 224 | 236 | 4 | 5 | 2 | 5 | 162 | 180 | 1 |
| 1 | 14 | 3 | 18 | 16 | 1 | -6 | 3 | 4 | 36 | 28 | 1 | 3 | 7 | 4 | 39 | 41 | 1 | 1 | 12 | 4 | 28 | 22 | 1 | 6 | 2 | 5 | 299 | 307 | 2 |
| 3 | 14 | 3 | 40 | 42 | 1 | -5 | 3 | 4 | 316 | 313 | 1 | 4 | 7 | 4 | 94 | 95 | 1 | 3 | 12 | 4 | 94 | 92 | 1 | 9 | 2 | 5 | 5 | 13 | 4 |
| 5 | 14 | 3 | 50 | 45 | 1 | -4 | 3 | 4 | 629 | 613 | 5 | 4 | 7 | 4 | 44 | 43 | 1 | 4 | 12 | 4 | 55 | 52 | 1 | -10 | 3 | 5 | 16 | 21 | 1 |
| -6 | 15 | 3 | 0 | 0 | 1 | -3 | 3 | 4 | 108 | 111 | 1 | 5 | 7 | 4 | 44 | 43 | 1 | 5 | 12 | 4 | 77 | 78 | 1 | -9 | 3 | 5 | 8 | 0 | 8 |
| -4 | 15 | 3 | 12 | 5 | 4 | -2 | 3 | 4 | 82 | 87 | 1 | 6 | 7 | 4 | 157 | 156 | 1 | 7 | 12 | 4 | 36 | 37 | 1 | -8 | 3 | 5 | 72 | 70 | 1 |
| -3 | 15 | 3 | 0 | 4 | 1 | 0 | 3 | 4 | 216 | 221 | 1 | 7 | 7 | 4 | 13 | 16 | 3 | 8 | 13 | 4 | 0 | 12 | 1 | -7 | 3 | 5 | 29 | 28 | 1 |
| -2 | 15 | 3 | 18 | 14 | 1 | 1 | 3 | 4 | 218 | 229 | 2 | 8 | 7 | 4 | 17 | 20 | 1 | -6 | 13 | 4 | 0 | 12 | 1 | -6 | 3 | 5 | 68 | 64 | 1 |
| 0 | 15 | 3 | 35 | 38 | 1 | 2 | 3 | 4 | 50 | 57 | 1 | 9 | 7 | 4 | 24 | 32 | 1 | -4 | 13 | 4 | 0 | 5 | 1 | -7 | 3 | 5 | 201 | 202 | 3 |
| 1 | 15 | 3 | 8 | 6 | 2 | 3 | 3 | 4 | 86 | 85 | 1 | -11 | 8 | 4 | 8 | 17 | 8 | -3 | 13 | 4 | 0 | 3 | 1 | -5 | 3 | 5 | 226 | 214 | 1 |
| 3 | 15 | 3 | 34 | 49 | 1 | 4 | 3 | 4 | 97 | 103 | 2 | -10 | 8 | 4 | 11 | 1 | 4 | -2 | 13 | 4 | 31 | 30 | 1 | -4 | 3 | 5 | 44 | 43 | 1 |
| 4 | 15 | 3 | 37 | 33 | 1 | 5 | 3 | 4 | 110 | 111 | 1 | -8 | 8 | 4 | 153 | 152 | 1 | -1 | 13 | 4 | 79 | 87 | 3 | -2 | 3 | 5 | 189 | 202 | 1 |
| 5 | 15 | 3 | 0 | 10 | 1 | 6 | 3 | 4 | 177 | 174 | 3 | -7 | 8 | 4 | 0 | 8 | 1 | 0 | 13 | 4 | 138 | 156 | 1 | -1 | 3 | 5 | 281 | 289 | 1 |
| 6 | 15 | 3 | 0 | 6 | 1 | 7 | 3 | 4 | 17 | 27 | 2 | -6 | 8 | 4 | 71 | 71 | 1 | 1 | 13 | 4 | 32 | 29 | 1 | -1 | 3 | 5 | 459 | 467 | 4 |
| -6 | 16 | 3 | 62 | 58 | 1 | 8 | 3 | 4 | 65 | 57 | 1 | -5 | 8 | 4 | 80 | 77 | 1 | 2 | 13 | 4 | 95 | 95 | 1 | 0 | 3 | 5 | 124 | 120 | 1 |
| -5 | 16 | 3 | 12 | 10 | 6 | 9 | 3 | 4 | 0 | 19 | 1 | -4 | 8 | 4 | 52 | 53 | 1 | 3 | 13 | 4 | 27 | 35 | 1 | 2 | 3 | 5 | 193 | 195 | 2 |
| -3 | 16 | 3 | 39 | 39 | 1 | -10 | 4 | 4 | 14 | 22 | 4 | -3 | 8 | 4 | 5 | 12 | 4 | 5 | 13 | 4 | 30 | 32 | 1 | 2 | 3 | 5 | 46 | 56 | 1 |
| -2 | 16 | 3 | 0 | 9 | 1 | -8 | 4 | 4 | 0 | 7 | 1 | -2 | 8 | 4 | 44 | 41 | 1 | -6 | 14 | 4 | 40 | 48 | 1 | 3 | 3 | 5 | 10 | 12 | 1 |
| -1 | 16 | 3 | 20 | 20 | 1 | -7 | 4 | 4 | 40 | 44 | 4 | -1 | 8 | 4 | 171 | 166 | 1 | -5 | 14 | 4 | 13 | 9 | 4 | 4 | 3 | 5 | 146 | 156 | 2 |
| 1 | 16 | 3 | 8 | 4 | 3 | -6 | 4 | 4 | 142 | 142 | 1 | 0 | 8 | 4 | 266 | 252 | 1 | -4 | 14 | 4 | 0 | 9 | 1 | 5 | 3 | 5 | 43 | 48 | 1 |
| 4 | 16 | 3 | 15 | 9 | 4 | -5 | 4 | 4 | 136 | 132 | 1 | 1 | 8 | 4 | 281 | 285 | 2 | -3 | 14 | 4 | 17 | 17 | 1 | 6 | 3 | 5 | 156 | 161 | 1 |
| -4 | 17 | 3 | 44 | 46 | 1 | -4 | 4 | 4 | 151 | 145 | 1 | 2 | 8 | 4 | 58 | 65 | 1 | -2 | 14 | 4 | 40 | 39 | 1 | 7 | 3 | 5 | 106 | 99 | 3 |
| -3 | 17 | 3 | 0 | 8 | 1 | -3 | 4 | 4 | 0 | 2 | 1 | 3 | 8 | 4 | 133 | 139 | 1 | -1 | 14 | 4 | 43 | 49 | 1 | 8 | 3 | 5 | 85 | 85 | 1 |
| -2 | 17 | 3 | 26 | 23 | 1 | -2 | 4 | 4 | 309 | 306 | 2 | 4 | 8 | 4 | 131 | 134 | 2 | 0 | 14 | 4 | 11 | 16 | 1 | 10 | 3 | 5 | 12 | 8 | 7 |
| 1 | 17 | 3 | 6 | 7 | 4 | -1 | 4 | 4 | 99 | 86 | 1 | 5 | 8 | 4 | 16 | 10 | 1 | 1 | 14 | 4 | 19 | 17 | 1 | -11 | 4 | 5 | 0 | 13 | 1 |
| 2 | 17 | 3 | 32 | 35 | 1 | 0 | 4 | 4 | 235 | 235 | 3 | 6 | 8 | 4 | 59 | 54 | 1 | 2 | 14 | 4 | 0 | 1 | 1 | -10 | 4 | 5 | 32 | 35 | 4 |
| 3 | 17 | 3 | 13 | 5 | 4 | 1 | 4 | 4 | 317 | 313 | 2 | 7 | 8 | 4 | 47 | 55 | 1 | 5 | 14 | 4 | 23 | 25 | 2 | -9 | 4 | 5 | 94 | 84 | 1 |
| -5 | 18 | 3 | 34 | 42 | 1 | 2 | 4 | 4 | 75 | 65 | 1 | 8 | 8 | 4 | 10 | 7 | 4 | -7 | 15 | 4 | 12 | 4 | 6 | -8 | 4 | 5 | 13 | 12 | 1 |
| -3 | 18 | 3 | 8 | 12 | 4 | 3 | 4 | 4 | 246 | 233 | 1 | -10 | 9 | 4 | 14 | 18 | 1 | -3 | 15 | 4 | 39 | 35 | 1 | -7 | 4 | 5 | 7 | 7 | 3 |
| 2 | 18 | 3 | 0 | 8 | 1 | 4 | 4 | 4 | 57 | 52 | 2 | -9 | 9 | 4 | 0 | 3 | 1 | -2 | 15 | 4 | 15 | 21 | 1 | -6 | 4 | 5 | 62 | 57 | 1 |
| 3 | 18 | 3 | 13 | 12 | 2 | 5 | 4 | 4 | 74 | 71 | 1 | -8 | 9 | 4 | 146 | 140 | 1 | -1 | 15 | 4 | 40 | 41 | 1 | -5 | 4 | 5 | 221 | 214 | 1 |
| 4 | 18 | 3 | 12 | 4 | 8 | 6 | 4 | 4 | 53 | 56 | 1 | -7 | 9 | 4 | 68 | 70 | 1 | 0 | 15 | 4 | 11 | 9 | 2 | -4 | 4 | 5 | 103 | 111 | 1 |
| -3 | 19 | 3 | 29 | 31 | 1 | 7 | 4 | 4 | 45 | 52 | 1 | -6 | 9 | 4 | 22 | 25 | 1 | 2 | 15 | 4 | 8 | 7 | 6 | -3 | 4 | 5 | 5 | 4 | 4 |
| 2 | 19 | 3 | 14 | 24 | 1 | 8 | 4 | 4 | | | | | | | | | | | | | | | | | | | | | |

Table 10.

Observed and calculated structure factors for pchm26

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|-----|---|---|------|------|-----|-----|----|---|------|------|-----|-----|----|---|------|------|-----|-----|---|---|------|------|-----|-----|----|---|------|------|-----|
| 7 | 5 | 5 | 0 | 10 | 1 | -5 | 10 | 5 | 62 | 67 | 1 | 2 | 17 | 5 | 0 | 18 | 1 | -4 | 4 | 6 | 181 | 177 | 2 | 5 | 8 | 6 | 50 | 49 | 1 |
| 8 | 5 | 5 | 40 | 42 | 2 | -4 | 10 | 5 | 94 | 94 | 4 | -5 | 18 | 5 | 9 | 15 | 9 | -3 | 4 | 6 | 39 | 41 | 1 | 6 | 8 | 6 | 32 | 36 | 1 |
| 9 | 5 | 5 | 34 | 37 | 1 | -2 | 10 | 5 | 52 | 53 | 1 | -3 | 18 | 5 | 28 | 30 | 1 | -2 | 4 | 6 | 169 | 166 | 1 | 7 | 8 | 6 | 31 | 28 | 1 |
| -12 | 6 | 5 | 32 | 36 | 2 | -1 | 10 | 5 | 0 | 4 | 1 | 1 | 18 | 5 | 24 | 31 | 1 | -1 | 4 | 6 | 418 | 420 | 2 | 8 | 8 | 6 | 11 | 5 | 3 |
| -11 | 6 | 5 | 16 | 28 | 3 | 0 | 10 | 5 | 61 | 58 | 1 | 2 | 18 | 5 | 11 | 18 | 4 | 0 | 4 | 6 | 107 | 119 | 1 | 9 | 8 | 6 | 8 | 6 | 8 |
| -10 | 6 | 5 | 53 | 53 | 2 | 1 | 10 | 5 | 32 | 36 | 1 | 3 | 18 | 5 | 19 | 26 | 3 | 1 | 4 | 6 | 212 | 202 | 2 | 10 | 8 | 6 | 65 | 56 | 1 |
| -9 | 6 | 5 | 69 | 63 | 1 | 2 | 10 | 5 | 9 | 13 | 1 | -4 | 19 | 5 | 10 | 6 | 3 | 2 | 4 | 6 | 29 | 26 | 1 | -12 | 9 | 6 | 65 | 53 | 1 |
| -8 | 6 | 5 | 96 | 103 | 1 | 4 | 10 | 5 | 69 | 66 | 1 | -3 | 19 | 5 | 6 | 8 | 6 | 3 | 4 | 6 | 74 | 69 | 1 | -10 | 9 | 6 | 48 | 45 | 1 |
| -7 | 6 | 5 | 81 | 90 | 1 | 5 | 10 | 5 | 65 | 62 | 1 | 2 | 19 | 5 | 25 | 33 | 1 | 4 | 4 | 6 | 87 | 90 | 2 | -9 | 9 | 6 | 26 | 27 | 1 |
| -6 | 6 | 5 | 81 | 84 | 1 | 6 | 10 | 5 | 55 | 51 | 1 | -11 | 0 | 6 | 113 | 102 | 1 | 5 | 4 | 6 | 101 | 96 | 1 | -8 | 9 | 6 | 62 | 62 | 1 |
| -5 | 6 | 5 | 102 | 96 | 1 | 7 | 10 | 5 | 12 | 15 | 1 | -10 | 0 | 6 | 8 | 14 | 8 | 6 | 4 | 6 | 298 | 284 | 2 | -7 | 9 | 6 | 32 | 28 | 1 |
| -4 | 6 | 5 | 128 | 123 | 1 | 8 | 10 | 5 | 9 | 5 | 5 | -9 | 0 | 6 | 40 | 32 | 1 | 7 | 4 | 6 | 0 | 12 | 1 | -6 | 9 | 6 | 85 | 79 | 1 |
| -3 | 6 | 5 | 168 | 175 | 1 | -11 | 11 | 5 | 0 | 11 | 1 | -8 | 0 | 6 | 378 | 377 | 4 | 8 | 4 | 6 | 57 | 54 | 1 | -5 | 9 | 6 | 99 | 95 | 1 |
| -2 | 6 | 5 | 254 | 252 | 3 | -10 | 11 | 5 | 14 | 13 | 2 | -7 | 0 | 6 | 113 | 110 | 1 | -10 | 5 | 6 | 68 | 69 | 1 | -4 | 9 | 6 | 272 | 270 | 1 |
| -1 | 6 | 5 | 222 | 216 | 3 | -9 | 11 | 5 | 76 | 72 | 1 | -6 | 0 | 6 | 67 | 73 | 1 | -9 | 5 | 6 | 47 | 52 | 1 | -3 | 9 | 6 | 32 | 30 | 1 |
| 0 | 6 | 5 | 136 | 126 | 1 | -8 | 11 | 5 | 74 | 72 | 1 | -5 | 0 | 6 | 67 | 74 | 1 | -8 | 5 | 6 | 172 | 175 | 2 | -2 | 9 | 6 | 11 | 13 | 1 |
| 1 | 6 | 5 | 136 | 133 | 2 | -7 | 11 | 5 | 9 | 10 | 1 | -4 | 0 | 6 | 200 | 214 | 1 | -7 | 5 | 6 | 24 | 28 | 1 | -1 | 9 | 6 | 36 | 37 | 1 |
| 2 | 6 | 5 | 69 | 64 | 1 | -4 | 11 | 5 | 81 | 89 | 1 | -3 | 0 | 6 | 89 | 103 | 1 | -6 | 5 | 6 | 70 | 66 | 1 | 0 | 9 | 6 | 242 | 252 | 3 |
| 3 | 6 | 5 | 230 | 214 | 1 | -3 | 11 | 5 | 155 | 153 | 1 | -2 | 0 | 6 | 205 | 186 | 1 | -5 | 5 | 6 | 205 | 213 | 1 | 1 | 9 | 6 | 95 | 89 | 2 |
| 4 | 6 | 5 | 41 | 37 | 2 | -2 | 11 | 5 | 62 | 63 | 1 | 0 | 0 | 6 | 276 | 277 | 2 | -4 | 5 | 6 | 290 | 287 | 1 | 3 | 9 | 6 | 137 | 134 | 2 |
| 5 | 6 | 5 | 53 | 54 | 2 | -1 | 11 | 5 | 15 | 20 | 1 | 1 | 0 | 6 | 24 | 26 | 1 | -3 | 5 | 6 | 333 | 323 | 2 | 4 | 9 | 6 | 162 | 167 | 15 |
| 6 | 6 | 5 | 87 | 84 | 6 | 0 | 11 | 5 | 163 | 168 | 3 | 2 | 0 | 6 | 46 | 47 | 1 | -2 | 5 | 6 | 86 | 79 | 1 | 5 | 9 | 6 | 54 | 50 | 1 |
| 7 | 6 | 5 | 37 | 40 | 1 | 1 | 11 | 5 | 10 | 8 | 1 | 3 | 0 | 6 | 290 | 286 | 2 | -1 | 5 | 6 | 252 | 250 | 2 | 6 | 9 | 6 | 8 | 0 | 3 |
| 8 | 6 | 5 | 28 | 28 | 1 | 2 | 11 | 5 | 137 | 131 | 1 | 4 | 0 | 6 | 27 | 25 | 1 | 0 | 5 | 6 | 272 | 262 | 1 | 7 | 9 | 6 | 22 | 22 | 1 |
| -10 | 7 | 5 | 22 | 18 | 2 | 3 | 11 | 5 | 32 | 36 | 1 | 5 | 0 | 6 | 104 | 100 | 1 | 1 | 5 | 6 | 113 | 114 | 1 | 8 | 9 | 6 | 17 | 22 | 1 |
| -9 | 7 | 5 | 61 | 59 | 1 | 4 | 11 | 5 | 131 | 139 | 1 | 6 | 0 | 6 | 301 | 296 | 2 | 2 | 5 | 6 | 19 | 22 | 1 | -11 | 10 | 6 | 20 | 21 | 2 |
| -8 | 7 | 5 | 152 | 159 | 1 | 5 | 11 | 5 | 9 | 9 | 3 | 7 | 0 | 6 | 57 | 52 | 1 | 3 | 5 | 6 | 26 | 27 | 1 | -10 | 10 | 6 | 11 | 8 | 3 |
| -6 | 7 | 5 | 16 | 23 | 3 | 6 | 11 | 5 | 14 | 9 | 8 | 8 | 0 | 6 | 12 | 20 | 5 | 4 | 5 | 6 | 17 | 20 | 1 | -9 | 10 | 6 | 53 | 47 | 5 |
| -5 | 7 | 5 | 132 | 122 | 1 | 7 | 11 | 5 | 18 | 14 | 1 | -10 | 1 | 6 | 0 | 5 | 1 | 5 | 5 | 6 | 95 | 96 | 1 | -8 | 10 | 6 | 0 | 3 | 1 |
| -4 | 7 | 5 | 58 | 58 | 1 | 8 | 11 | 5 | 0 | 9 | 1 | -8 | 1 | 6 | 173 | 192 | 3 | 6 | 5 | 6 | 260 | 252 | 2 | -7 | 10 | 6 | 0 | 2 | 1 |
| -3 | 7 | 5 | 48 | 59 | 1 | -6 | 12 | 5 | 19 | 31 | 3 | -7 | 1 | 6 | 69 | 75 | 1 | 7 | 5 | 6 | 99 | 104 | 1 | -6 | 10 | 6 | 9 | 1 | 3 |
| -2 | 7 | 5 | 5 | 4 | 2 | -5 | 12 | 5 | 84 | 74 | 1 | -6 | 1 | 6 | 127 | 125 | 1 | 8 | 5 | 6 | 14 | 9 | 4 | -5 | 10 | 6 | 96 | 89 | 1 |
| -1 | 7 | 5 | 65 | 75 | 1 | -3 | 12 | 5 | 33 | 36 | 1 | -5 | 1 | 6 | 71 | 65 | 1 | -11 | 6 | 6 | 0 | 5 | 1 | -4 | 10 | 6 | 119 | 128 | 3 |
| 0 | 7 | 5 | 226 | 213 | 1 | -2 | 12 | 5 | 137 | 135 | 1 | -4 | 1 | 6 | 142 | 131 | 4 | -10 | 6 | 6 | 13 | 19 | 2 | -3 | 10 | 6 | 129 | 135 | 2 |
| 1 | 7 | 5 | 43 | 43 | 1 | -1 | 12 | 5 | 53 | 55 | 1 | -3 | 1 | 6 | 308 | 310 | 2 | -9 | 6 | 6 | 134 | 130 | 1 | -2 | 10 | 6 | 47 | 55 | 1 |
| 2 | 7 | 5 | 194 | 190 | 1 | 0 | 12 | 5 | 14 | 22 | 4 | -2 | 1 | 6 | 166 | 169 | 1 | -8 | 6 | 6 | 47 | 50 | 1 | -1 | 10 | 6 | 87 | 80 | 2 |
| 3 | 7 | 5 | 224 | 219 | 2 | 1 | 12 | 5 | 98 | 89 | 1 | -1 | 1 | 6 | 578 | 569 | 3 | -7 | 6 | 6 | 43 | 46 | 1 | 0 | 10 | 6 | 105 | 99 | 1 |
| 4 | 7 | 5 | 44 | 50 | 1 | 2 | 12 | 5 | 45 | 41 | 1 | 0 | 1 | 6 | 110 | 103 | 1 | -6 | 6 | 6 | 112 | 111 | 1 | 1 | 10 | 6 | 58 | 65 | 1 |
| 5 | 7 | 5 | 114 | 114 | 1 | 3 | 12 | 5 | 13 | 6 | 3 | 1 | 1 | 6 | 240 | 239 | 1 | -5 | 6 | 6 | 94 | 95 | 1 | 2 | 10 | 6 | 96 | 98 | 3 |
| 6 | 7 | 5 | 49 | 41 | 1 | 5 | 12 | 5 | 16 | 23 | 4 | 2 | 1 | 6 | 51 | 52 | 1 | -4 | 6 | 6 | 147 | 141 | 1 | 4 | 10 | 6 | 60 | 56 | 1 |
| 7 | 7 | 5 | 78 | 72 | 1 | -7 | 13 | 5 | 40 | 43 | 1 | 3 | 1 | 6 | 89 | 93 | 1 | -3 | 6 | 6 | 155 | 155 | 1 | 5 | 10 | 6 | 16 | 16 | 5 |
| 8 | 7 | 5 | 9 | 4 | 7 | -4 | 13 | 5 | 0 | 6 | 1 | 4 | 1 | 6 | 21 | 22 | 1 | -2 | 6 | 6 | 39 | 31 | 1 | 6 | 10 | 6 | 19 | 9 | 1 |
| 10 | 7 | 5 | 23 | 23 | 3 | -3 | 13 | 5 | 30 | 29 | 1 | 5 | 1 | 6 | 173 | 173 | 3 | -1 | 6 | 6 | 114 | 112 | 1 | 9 | 10 | 6 | 11 | 16 | 7 |
| -10 | 8 | 5 | 19 | 15 | 2 | -2 | 13 | 5 | 66 | 68 | 1 | 6 | 1 | 6 | 44 | 46 | 1 | 0 | 6 | 6 | 66 | 67 | 1 | -11 | 11 | 6 | 95 | 83 | 1 |
| -9 | 8 | 5 | 43 | 45 | 1 | -1 | 13 | 5 | 85 | 91 | 1 | 7 | 1 | 6 | 50 | 49 | 1 | 1 | 6 | 6 | 177 | 184 | 1 | -10 | 11 | 6 | 71 | 62 | 1 |
| -8 | 8 | 5 | 41 | 51 | 1 | 0 | 13 | 5 | 11 | 18 | 3 | -11 | 2 | 6 | 17 | 21 | 2 | 2 | 6 | 6 | 58 | 55 | 1 | -9 | 11 | 6 | 0 | 3 | 1 |
| -7 | 8 | 5 | 14 | 21 | 1 | 1 | 13 | 5 | 10 | 7 | 2 | -10 | 2 | 6 | 81 | 82 | 1 | 3 | 6 | 6 | 269 | 263 | 3 | -8 | 11 | 6 | 7 | 3 | 3 |
| -6 | 8 | 5 | 0 | 4 | 1 | 3 | 13 | 5 | 93 | 91 | 1 | -9 | 2 | 6 | 90 | 88 | 1 | 4 | 6 | 6 | 55 | 51 | 1 | -7 | 11 | 6 | 15 | 15 | 4 |
| -5 | 8 | 5 | 13 | 9 | 1 | 4 | 13 | 5 | 78 | 69 | 1 | -8 | 2 | 6 | 207 | 209 | 5 | 5 | 6 | 6 | 10 | 1 | 2 | -6 | 11 | 6 | 67 | 67 | 1 |
| -4 | 8 | 5 | 129 | 140 | 1 | 5 | 13 | 5 | 41 | 40 | 1 | -7 | 2 | 6 | 24 | 29 | 1 | 6 | 6 | 6 | 19 | 22 | 1 | -5 | 11 | 6 | 10 | 10 | 3 |
| -3 | 8 | 5 | 84 | 85 | 1 | -7 | 14 | 5 | 69 | 59 | 1 | -6 | 2 | 6 | 44 | 45 | 1 | 7 | 6 | 6 | 11 | 14 | 5 | -4 | 11 | 6 | 177 | 180 | 1 |
| -2 | 8 | 5 | 146 | 152 | 1 | -5 | 14 | 5 | 0 | 13 | 1 | -5 | 2 | 6 | 256 | 268 | 3 | 8 | 6 | 6 | 0 | 9 | 1 | -3 | 11 | 6 | 109 | 104 | 1 |
| -1 | 8 | 5 | 96 | 92 | 1 | -3 | 14 | 5 | 93 | 89 | 1 | -4 | 2 | 6 | 56 | 54 | 1 | -11 | 7 | 6 | 12 | 13 | 2 | -2 | 11 | 6 | 120 | 126 | 2 |
| 0 | 8 | 5 | 161 | 156 | 1 | -2 | 14 | 5 | 78 | 68 | 1 | -3 | 2 | 6 | 112 | 103 | 1 | -10 | 7 | 6 | 49 | 50 | 1 | -1 | 11 | 6 | 77 | 75 | 1 |
| 1 | 8 | 5 | 160 | 154 | 1 | -1 | 14 | 5 | 41 | 43 | 1 | -2 | 2 | 6 | 119 | 122 | 1 | -9 | 7 | 6 | 8 | 6 | 4 | 0 | 11 | 6 | 23 | 28 | 1 |
| 2 | 8 | 5 | 138 | 138 | 1 | 0 | 14 | 5 | 61 | 55 | 1 | 0 | 2 | 6 | 180 | 166 | 1 | -8 | 7 | 6 | 104 | 102 | 1 | 1 | 11 | 6 | 117 | 112 | 1 |
| 3 | 8 | 5 | 27 | 25 | 1 | 1 | 14 | 5 | 10 | 13 | 2 | 1 | 2 | 6 | 397 | 383 | 2 | -7 | 7 | 6 | 8 | 5 | 4 | 2 | 11 | 6 | 87 | 90 | 1 |
| 4 | 8 | 5 | 0 | 3 | 1 | 2 | 14 | 5 | 85 | 83 | 1 | 2 | 2 | 6 | 270 | 269 | 1 | -6 | 7 | 6 | 64 | 75 | 2 | 3 | 11 | 6 | 59 | 66 | 7 |
| 5 | 8 | 5 | 52 | 55 | 1 | 3 | 14 | 5 | 22 | 24 | 2 | 3 | 2 | 6 | 33 | 23 | 1 | -5 | 7 | 6 | 121 | 127 | 1 | 4 | 11 | 6 | 11 | 13 | 2 |
| 6 | 8 | 5 | 42 | 41 | 1 | 5 | 14 | 5 | 63 | 60 | 1 | 4 | 2 | 6 | 6 | 8 | 5 | -4 | 7 | 6 | 242 | 241 | 1 | 5 | 11 | 6 | 55 | 50 | 1 |
| 7 | 8 | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

Table 10. Observed and calculated structure factors for pchm26

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | | | | | | |
|-----|----|---|------|------|-----|-----|---|---|------|------|-----|-----|----|---|------|------|-----|----|----|---|------|------|-----|-----|---|---|-----|-----|----|
| 3 | 13 | 6 | 119 | 112 | 1 | -3 | 3 | 7 | 257 | 265 | 2 | -8 | 8 | 7 | 43 | 47 | 1 | 8 | 12 | 7 | 10 | 13 | 3 | 2 | 1 | 8 | 137 | 138 | 1 |
| 4 | 13 | 6 | 14 | 15 | 4 | -2 | 3 | 7 | 285 | 274 | 1 | -7 | 8 | 7 | 10 | 9 | 2 | -6 | 13 | 7 | 13 | 1 | 5 | 3 | 1 | 8 | 49 | 47 | 2 |
| 6 | 13 | 6 | 30 | 27 | 2 | -1 | 3 | 7 | 572 | 558 | 3 | -6 | 8 | 7 | 181 | 183 | 1 | -5 | 13 | 7 | 6 | 3 | 6 | 4 | 1 | 8 | 57 | 65 | 1 |
| -7 | 14 | 6 | 13 | 10 | 7 | 0 | 3 | 7 | 9 | 9 | 5 | -5 | 8 | 7 | 187 | 185 | 2 | -4 | 13 | 7 | 32 | 31 | 1 | 5 | 1 | 8 | 49 | 47 | 2 |
| -6 | 14 | 6 | 33 | 34 | 7 | 1 | 3 | 7 | 169 | 173 | 1 | -4 | 8 | 7 | 7 | 2 | 7 | -3 | 13 | 7 | 10 | 7 | 1 | 6 | 1 | 8 | 33 | 39 | 1 |
| -5 | 14 | 6 | 96 | 107 | 1 | 2 | 3 | 7 | 65 | 67 | 1 | -3 | 8 | 7 | 89 | 84 | 1 | -2 | 13 | 7 | 11 | 5 | 1 | 7 | 1 | 8 | 52 | 52 | 2 |
| -4 | 14 | 6 | 42 | 36 | 1 | 3 | 3 | 7 | 110 | 112 | 1 | -2 | 8 | 7 | 164 | 163 | 1 | -1 | 13 | 7 | 18 | 13 | 3 | 8 | 1 | 8 | 12 | 17 | 3 |
| -3 | 14 | 6 | 0 | 0 | 1 | 4 | 3 | 7 | 169 | 164 | 2 | -1 | 8 | 7 | 143 | 136 | 1 | 0 | 13 | 7 | 0 | 11 | 1 | 9 | 1 | 8 | 48 | 45 | 1 |
| -2 | 14 | 6 | 26 | 30 | 7 | 5 | 3 | 7 | 57 | 52 | 1 | 0 | 8 | 7 | 81 | 81 | 1 | 1 | 13 | 7 | 7 | 5 | 3 | -9 | 2 | 8 | 19 | 11 | 1 |
| -1 | 14 | 6 | 76 | 74 | 3 | 7 | 3 | 7 | 115 | 110 | 1 | 1 | 8 | 7 | 77 | 78 | 1 | 2 | 13 | 7 | 45 | 64 | 37 | -8 | 2 | 8 | 30 | 28 | 1 |
| 0 | 14 | 6 | 42 | 41 | 1 | 8 | 3 | 7 | 37 | 38 | 1 | 2 | 8 | 7 | 189 | 185 | 2 | 3 | 13 | 7 | 31 | 34 | 19 | -7 | 2 | 8 | 28 | 31 | 1 |
| 1 | 14 | 6 | 10 | 3 | 5 | 9 | 3 | 7 | 20 | 22 | 2 | 3 | 8 | 7 | 122 | 124 | 1 | 4 | 13 | 7 | 14 | 24 | 4 | -6 | 2 | 8 | 131 | 135 | 1 |
| 3 | 14 | 6 | 77 | 69 | 1 | -12 | 4 | 7 | 45 | 42 | 1 | 4 | 8 | 7 | 10 | 12 | 2 | 7 | 13 | 7 | 24 | 27 | 1 | -5 | 2 | 8 | 85 | 87 | 1 |
| -7 | 15 | 6 | 16 | 17 | 7 | -8 | 4 | 7 | 85 | 89 | 3 | 5 | 8 | 7 | 15 | 21 | 1 | -6 | 14 | 7 | 13 | 15 | 6 | -4 | 2 | 8 | 15 | 19 | 3 |
| -5 | 15 | 6 | 20 | 24 | 1 | -7 | 4 | 7 | 12 | 8 | 1 | 7 | 8 | 7 | 26 | 26 | 1 | -4 | 14 | 7 | 53 | 51 | 1 | -3 | 2 | 8 | 402 | 402 | 3 |
| -4 | 15 | 6 | 0 | 4 | 1 | -6 | 4 | 7 | 66 | 63 | 1 | 8 | 8 | 7 | 0 | 8 | 1 | -3 | 14 | 7 | 18 | 30 | 17 | -2 | 2 | 8 | 90 | 91 | 1 |
| -2 | 15 | 6 | 40 | 39 | 1 | -5 | 4 | 7 | 14 | 22 | 2 | 9 | 8 | 7 | 59 | 52 | 1 | -2 | 14 | 7 | 24 | 25 | 1 | -1 | 2 | 8 | 253 | 256 | 1 |
| -1 | 15 | 6 | 45 | 45 | 2 | -4 | 4 | 7 | 106 | 116 | 2 | -10 | 9 | 7 | 0 | 0 | 1 | -1 | 14 | 7 | 13 | 7 | 1 | 0 | 2 | 8 | 201 | 210 | 1 |
| 0 | 15 | 6 | 22 | 24 | 1 | -3 | 4 | 7 | 187 | 182 | 1 | -9 | 9 | 7 | 84 | 76 | 5 | 0 | 14 | 7 | 10 | 5 | 2 | 1 | 2 | 8 | 262 | 254 | 1 |
| 1 | 15 | 6 | 52 | 54 | 1 | -2 | 4 | 7 | 75 | 70 | 1 | -8 | 9 | 7 | 87 | 92 | 1 | 1 | 14 | 7 | 10 | 17 | 1 | 2 | 2 | 8 | 237 | 226 | 3 |
| 2 | 15 | 6 | 35 | 40 | 1 | -1 | 4 | 7 | 67 | 58 | 1 | -7 | 9 | 7 | 67 | 73 | 2 | 2 | 14 | 7 | 17 | 18 | 3 | 3 | 2 | 8 | 198 | 195 | 1 |
| 3 | 15 | 6 | 13 | 6 | 5 | 0 | 4 | 7 | 71 | 82 | 1 | -6 | 9 | 7 | 18 | 22 | 3 | 3 | 14 | 7 | 27 | 26 | 1 | 4 | 2 | 8 | 124 | 122 | 1 |
| -7 | 16 | 6 | 0 | 9 | 1 | 1 | 4 | 7 | 102 | 106 | 1 | -5 | 9 | 7 | 10 | 1 | 2 | 5 | 14 | 7 | 0 | 7 | 1 | 5 | 2 | 8 | 32 | 30 | 1 |
| -5 | 16 | 6 | 61 | 56 | 1 | 2 | 4 | 7 | 83 | 86 | 1 | -4 | 9 | 7 | 146 | 144 | 1 | -7 | 15 | 7 | 23 | 24 | 2 | 6 | 2 | 8 | 60 | 59 | 1 |
| -4 | 16 | 6 | 57 | 48 | 1 | 3 | 4 | 7 | 25 | 27 | 1 | -3 | 9 | 7 | 70 | 74 | 1 | -6 | 15 | 7 | 14 | 3 | 3 | 7 | 2 | 8 | 14 | 8 | 10 |
| -3 | 16 | 6 | 0 | 3 | 1 | 4 | 4 | 7 | 7 | 1 | 3 | -2 | 9 | 7 | 229 | 229 | 1 | -4 | 15 | 7 | 72 | 63 | 1 | -10 | 3 | 8 | 16 | 16 | 2 |
| -2 | 16 | 6 | 0 | 0 | 1 | 5 | 4 | 7 | 27 | 23 | 1 | -1 | 9 | 7 | 51 | 61 | 1 | -3 | 15 | 7 | 17 | 12 | 1 | -9 | 3 | 8 | 190 | 188 | 6 |
| -1 | 16 | 6 | 18 | 25 | 1 | 6 | 4 | 7 | 16 | 21 | 3 | 0 | 9 | 7 | 7 | 14 | 6 | -2 | 15 | 7 | 7 | 2 | 4 | -8 | 3 | 8 | 82 | 91 | 1 |
| 0 | 16 | 6 | 18 | 21 | 1 | 7 | 4 | 7 | 68 | 63 | 1 | 1 | 9 | 7 | 77 | 77 | 1 | -1 | 15 | 7 | 10 | 1 | 1 | -7 | 3 | 8 | 233 | 232 | 4 |
| 1 | 16 | 6 | 8 | 1 | 3 | 10 | 4 | 7 | 57 | 62 | 1 | 2 | 9 | 7 | 50 | 48 | 1 | 0 | 15 | 7 | 48 | 48 | 1 | -6 | 3 | 8 | 56 | 54 | 1 |
| -4 | 17 | 6 | 12 | 19 | 4 | -11 | 5 | 7 | 0 | 15 | 1 | 3 | 9 | 7 | 106 | 112 | 1 | 2 | 15 | 7 | 10 | 6 | 4 | -5 | 3 | 8 | 35 | 36 | 1 |
| -3 | 17 | 6 | 0 | 11 | 1 | -10 | 5 | 7 | 13 | 9 | 4 | 4 | 9 | 7 | 140 | 130 | 1 | 3 | 15 | 7 | 15 | 14 | 4 | -4 | 3 | 8 | 70 | 63 | 1 |
| -2 | 17 | 6 | 42 | 43 | 1 | -9 | 5 | 7 | 72 | 70 | 1 | 5 | 9 | 7 | 78 | 77 | 1 | -7 | 16 | 7 | 0 | 0 | 1 | -3 | 3 | 8 | 572 | 577 | 7 |
| 1 | 17 | 6 | 12 | 13 | 3 | -8 | 5 | 7 | 183 | 183 | 1 | 6 | 9 | 7 | 15 | 9 | 2 | -6 | 16 | 7 | 53 | 46 | 1 | -2 | 3 | 8 | 71 | 72 | 1 |
| 3 | 17 | 6 | 50 | 55 | 1 | -7 | 5 | 7 | 78 | 77 | 1 | 8 | 9 | 7 | 19 | 19 | 1 | -5 | 16 | 7 | 53 | 56 | 1 | -1 | 3 | 8 | 559 | 542 | 3 |
| 4 | 17 | 6 | 13 | 10 | 7 | -6 | 5 | 7 | 109 | 106 | 1 | -12 | 10 | 7 | 65 | 58 | 1 | -4 | 16 | 7 | 0 | 8 | 1 | 0 | 3 | 8 | 255 | 242 | 1 |
| -5 | 18 | 6 | 43 | 37 | 1 | -5 | 5 | 7 | 50 | 53 | 1 | -11 | 10 | 7 | 8 | 6 | 8 | -3 | 16 | 7 | 0 | 1 | 1 | 1 | 3 | 8 | 165 | 163 | 1 |
| -3 | 18 | 6 | 39 | 41 | 1 | -4 | 5 | 7 | 102 | 104 | 1 | -9 | 10 | 7 | 39 | 38 | 1 | -2 | 16 | 7 | 24 | 26 | 1 | 2 | 3 | 8 | 9 | 6 | 2 |
| -2 | 18 | 6 | 9 | 0 | 1 | -3 | 5 | 7 | 152 | 156 | 1 | -8 | 10 | 7 | 73 | 69 | 1 | -1 | 16 | 7 | 12 | 15 | 2 | 3 | 3 | 8 | 183 | 175 | 2 |
| 1 | 18 | 6 | 0 | 3 | 1 | -2 | 5 | 7 | 262 | 264 | 3 | -7 | 10 | 7 | 42 | 40 | 1 | 0 | 16 | 7 | 5 | 1 | 5 | 4 | 3 | 8 | 103 | 103 | 1 |
| 2 | 18 | 6 | 0 | 5 | 1 | -1 | 5 | 7 | 120 | 118 | 1 | -6 | 10 | 7 | 115 | 109 | 1 | 1 | 16 | 7 | 18 | 22 | 2 | 5 | 3 | 8 | 10 | 8 | 2 |
| 1 | 19 | 6 | 12 | 17 | 3 | 0 | 5 | 7 | 204 | 195 | 1 | -4 | 10 | 7 | 25 | 26 | 1 | 2 | 16 | 7 | 15 | 14 | 3 | 6 | 3 | 8 | 104 | 112 | 1 |
| -10 | 1 | 7 | 47 | 48 | 1 | 1 | 5 | 7 | 131 | 128 | 1 | -3 | 10 | 7 | 141 | 144 | 1 | 4 | 16 | 7 | 24 | 21 | 3 | 7 | 3 | 8 | 31 | 43 | 1 |
| -9 | 1 | 7 | 18 | 18 | 1 | 2 | 5 | 7 | 113 | 115 | 1 | -2 | 10 | 7 | 123 | 122 | 1 | -6 | 17 | 7 | 18 | 23 | 3 | 8 | 3 | 8 | 0 | 4 | 1 |
| -8 | 1 | 7 | 0 | 9 | 1 | 3 | 5 | 7 | 40 | 44 | 2 | -1 | 10 | 7 | 474 | 470 | 5 | -4 | 17 | 7 | 40 | 39 | 1 | -12 | 4 | 8 | 12 | 1 | 6 |
| -7 | 1 | 7 | 127 | 132 | 1 | 4 | 5 | 7 | 10 | 9 | 2 | 0 | 10 | 7 | 7 | 10 | 7 | -3 | 17 | 7 | 20 | 23 | 1 | -11 | 4 | 8 | 0 | 5 | 1 |
| -6 | 1 | 7 | 68 | 67 | 1 | 5 | 5 | 7 | 14 | 8 | 2 | 1 | 10 | 7 | 51 | 50 | 1 | -2 | 17 | 7 | 24 | 22 | 1 | -10 | 4 | 8 | 44 | 48 | 1 |
| -5 | 1 | 7 | 259 | 254 | 5 | 6 | 5 | 7 | 19 | 55 | 1 | 2 | 10 | 7 | 21 | 16 | 1 | -1 | 17 | 7 | 12 | 21 | 1 | -9 | 4 | 8 | 57 | 45 | 1 |
| -4 | 1 | 7 | 501 | 496 | 3 | 7 | 5 | 7 | 19 | 25 | 1 | 3 | 10 | 7 | 96 | 91 | 1 | 0 | 17 | 7 | 6 | 5 | 6 | -8 | 4 | 8 | 159 | 148 | 1 |
| -3 | 1 | 7 | 71 | 71 | 1 | 8 | 5 | 7 | 0 | 9 | 1 | 4 | 10 | 7 | 54 | 52 | 2 | 2 | 17 | 7 | 8 | 6 | 7 | -7 | 4 | 8 | 58 | 53 | 1 |
| -2 | 1 | 7 | 53 | 43 | 1 | -9 | 6 | 7 | 8 | 20 | 8 | 5 | 10 | 7 | 20 | 19 | 1 | 3 | 17 | 7 | 45 | 44 | 1 | -6 | 4 | 8 | 44 | 45 | 1 |
| -1 | 1 | 7 | 245 | 253 | 1 | -8 | 6 | 7 | 96 | 89 | 1 | 6 | 10 | 7 | 135 | 122 | 1 | 4 | 17 | 7 | 0 | 4 | 1 | -5 | 4 | 8 | 99 | 106 | 1 |
| 0 | 1 | 7 | 126 | 130 | 1 | -7 | 6 | 7 | 23 | 17 | 7 | 9 | 10 | 7 | 17 | 9 | 4 | -5 | 18 | 7 | 0 | 2 | 1 | -4 | 4 | 8 | 265 | 270 | 3 |
| 1 | 1 | 7 | 145 | 142 | 2 | -6 | 6 | 7 | 64 | 63 | 1 | -11 | 11 | 7 | 41 | 46 | 1 | -4 | 18 | 7 | 23 | 27 | 2 | -3 | 4 | 8 | 68 | 73 | 1 |
| 2 | 1 | 7 | 121 | 115 | 1 | -5 | 6 | 7 | 116 | 116 | 2 | -10 | 11 | 7 | 13 | 15 | 2 | -3 | 18 | 7 | 21 | 22 | 2 | -2 | 4 | 8 | 65 | 67 | 1 |
| 3 | 1 | 7 | 381 | 369 | 2 | -4 | 6 | 7 | 65 | 63 | 1 | -9 | 11 | 7 | 20 | 16 | 1 | -2 | 18 | 7 | 22 | 27 | 1 | -1 | 4 | 8 | 39 | 46 | 1 |
| 4 | 1 | 7 | 0 | 11 | 1 | -3 | 6 | 7 | 151 | 149 | 1 | -8 | 11 | 7 | 22 | 14 | 6 | 0 | 18 | 7 | 0 | 0 | 1 | 0 | 4 | 8 | 69 | 74 | 2 |
| 5 | 1 | 7 | 63 | 62 | 1 | -2 | 6 | 7 | 237 | 245 | 1 | -7 | 11 | 7 | 10 | 4 | 4 | -3 | 19 | 7 | 5 | 2 | 5 | 1 | 4 | 8 | 70 | 73 | 1 |
| 6 | 1 | 7 | 74 | 72 | 1 | -1 | 6 | 7 | 371 | 369 | 6 | -6 | 11 | 7 | 56 | 66 | 7 | 1 | 19 | 7 | 0 | 8 | 1 | 2 | 4 | 8 | 164 | 155 | 1 |
| 7 | 1 | 7 | 11 | 11 | 8 | 0 | 6 | 7 | 76 | 78 | 1 | -5 | 11 | 7 | 110 | 106 | 1 | -9 | 0 | 8 | 96 | 96 | 1 | 3 | 4 | 8 | 107 | 107 | 2 |
| 8 | 1 | 7 | 33 | 31 | 1 | 1 | 6 | 7 | 183 | 175 | 1 | -4 | 11 | 7 | 103 | 97 | 1 | | | | | | | | | | | | |

Table 10.

Observed and calculated structure factors for pchm26

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|-----|---|---|------|------|-----|-----|----|---|------|------|-----|-----|----|---|------|------|-----|-----|---|---|------|------|-----|-----|----|---|------|------|-----|
| -7 | 6 | 8 | 53 | 60 | 1 | 3 | 10 | 8 | 59 | 62 | 2 | -2 | 17 | 8 | 26 | 30 | 1 | -10 | 5 | 9 | 18 | 13 | 1 | 0 | 9 | 9 | 37 | 36 | 1 |
| -6 | 6 | 8 | 94 | 89 | 1 | 4 | 10 | 8 | 46 | 47 | 1 | 0 | 17 | 8 | 23 | 36 | 1 | -9 | 5 | 9 | 109 | 105 | 1 | 1 | 9 | 9 | 53 | 58 | 1 |
| -5 | 6 | 8 | 130 | 131 | 1 | 5 | 10 | 8 | 24 | 25 | 1 | 1 | 17 | 8 | 0 | 9 | 1 | -8 | 5 | 9 | 0 | 8 | 1 | 2 | 9 | 9 | 114 | 110 | 3 |
| -4 | 6 | 8 | 48 | 54 | 1 | 6 | 10 | 8 | 75 | 69 | 1 | 2 | 17 | 8 | 21 | 19 | 2 | -7 | 5 | 9 | 24 | 25 | 1 | 3 | 9 | 9 | 9 | 1 | 5 |
| -3 | 6 | 8 | 112 | 103 | 1 | 7 | 10 | 8 | 0 | 3 | 1 | 3 | 17 | 8 | 14 | 17 | 8 | -6 | 5 | 9 | 64 | 63 | 1 | 4 | 9 | 9 | 27 | 29 | 1 |
| -2 | 6 | 8 | 86 | 84 | 1 | 8 | 10 | 8 | 20 | 31 | 1 | -5 | 18 | 8 | 14 | 5 | 3 | -5 | 5 | 9 | 206 | 199 | 1 | 5 | 9 | 9 | 10 | 1 | 3 |
| -1 | 6 | 8 | 267 | 261 | 1 | -11 | 11 | 8 | 15 | 18 | 3 | -4 | 18 | 8 | 22 | 23 | 2 | -4 | 5 | 9 | 159 | 163 | 2 | 6 | 9 | 9 | 24 | 21 | 1 |
| 0 | 6 | 8 | 31 | 29 | 1 | -10 | 11 | 8 | 26 | 28 | 1 | -2 | 18 | 8 | 12 | 18 | 1 | -3 | 5 | 9 | 121 | 119 | 1 | 7 | 9 | 9 | 35 | 34 | 1 |
| 1 | 6 | 8 | 66 | 65 | 1 | -9 | 11 | 8 | 10 | 7 | 2 | -1 | 18 | 8 | 13 | 14 | 2 | -2 | 5 | 9 | 334 | 328 | 2 | 8 | 9 | 9 | 13 | 18 | 5 |
| 2 | 6 | 8 | 37 | 35 | 1 | -8 | 11 | 8 | 48 | 44 | 1 | 1 | 18 | 8 | 0 | 12 | 1 | -1 | 5 | 9 | 172 | 169 | 1 | -11 | 10 | 9 | 48 | 45 | 1 |
| 3 | 6 | 8 | 40 | 32 | 1 | -7 | 11 | 8 | 39 | 42 | 4 | 2 | 18 | 8 | 19 | 13 | 3 | 0 | 5 | 9 | 262 | 254 | 1 | -10 | 10 | 9 | 28 | 32 | 1 |
| 4 | 6 | 8 | 134 | 136 | 1 | -6 | 11 | 8 | 39 | 41 | 1 | -12 | 1 | 9 | 28 | 28 | 2 | 1 | 5 | 9 | 94 | 96 | 1 | -9 | 10 | 9 | 54 | 51 | 1 |
| 5 | 6 | 8 | 164 | 147 | 1 | -5 | 11 | 8 | 28 | 27 | 2 | -8 | 1 | 9 | 123 | 120 | 1 | 2 | 5 | 9 | 331 | 325 | 2 | -8 | 10 | 9 | 10 | 9 | 2 |
| 6 | 6 | 8 | 51 | 50 | 4 | -4 | 11 | 8 | 24 | 29 | 3 | -7 | 1 | 9 | 27 | 28 | 1 | 3 | 5 | 9 | 237 | 239 | 2 | -7 | 10 | 9 | 49 | 51 | 1 |
| 7 | 6 | 8 | 71 | 70 | 1 | -3 | 11 | 8 | 13 | 15 | 1 | -6 | 1 | 9 | 78 | 84 | 1 | 4 | 5 | 9 | 110 | 108 | 7 | -6 | 10 | 9 | 69 | 66 | 1 |
| -11 | 7 | 8 | 14 | 17 | 4 | -2 | 11 | 8 | 24 | 27 | 1 | -5 | 1 | 9 | 88 | 82 | 2 | 5 | 5 | 9 | 25 | 25 | 2 | -5 | 10 | 9 | 59 | 56 | 1 |
| -10 | 7 | 8 | 0 | 1 | 1 | -1 | 11 | 8 | 109 | 112 | 1 | -4 | 1 | 9 | 131 | 127 | 1 | 6 | 5 | 9 | 81 | 82 | 4 | -4 | 10 | 9 | 6 | 3 | 6 |
| -9 | 7 | 8 | 13 | 4 | 2 | 0 | 11 | 8 | 61 | 63 | 1 | -3 | 1 | 9 | 6 | 9 | 3 | 7 | 5 | 9 | 51 | 49 | 1 | -3 | 10 | 9 | 147 | 140 | 1 |
| -8 | 7 | 8 | 24 | 26 | 1 | 1 | 11 | 8 | 24 | 20 | 1 | -2 | 1 | 9 | 178 | 178 | 1 | 8 | 5 | 9 | 18 | 16 | 2 | -2 | 10 | 9 | 6 | 3 | 3 |
| -7 | 7 | 8 | 12 | 12 | 5 | 2 | 11 | 8 | 14 | 16 | 1 | -1 | 1 | 9 | 315 | 327 | 3 | -11 | 6 | 9 | 9 | 9 | 7 | -1 | 10 | 9 | 121 | 118 | 1 |
| -6 | 7 | 8 | 65 | 63 | 1 | 3 | 11 | 8 | 84 | 87 | 1 | 0 | 1 | 9 | 28 | 34 | 2 | -10 | 6 | 9 | 26 | 27 | 1 | 0 | 10 | 9 | 180 | 181 | 1 |
| -4 | 7 | 8 | 143 | 142 | 1 | 4 | 11 | 8 | 7 | 10 | 6 | 1 | 1 | 9 | 61 | 65 | 1 | -9 | 6 | 9 | 13 | 18 | 2 | 1 | 10 | 9 | 63 | 62 | 1 |
| -3 | 7 | 8 | 6 | 6 | 6 | 5 | 11 | 8 | 33 | 37 | 2 | 2 | 1 | 9 | 245 | 246 | 1 | -8 | 6 | 9 | 97 | 97 | 1 | 2 | 10 | 9 | 12 | 5 | 5 |
| -2 | 7 | 8 | 37 | 39 | 1 | 6 | 11 | 8 | 77 | 69 | 1 | 3 | 1 | 9 | 151 | 156 | 1 | -7 | 6 | 9 | 11 | 14 | 1 | 3 | 10 | 9 | 18 | 25 | 2 |
| -1 | 7 | 8 | 98 | 100 | 1 | 8 | 11 | 8 | 0 | 0 | 1 | 4 | 1 | 9 | 115 | 113 | 2 | -6 | 6 | 9 | 108 | 98 | 1 | 4 | 10 | 9 | 47 | 44 | 1 |
| 0 | 7 | 8 | 94 | 99 | 1 | -11 | 12 | 8 | 14 | 16 | 2 | 5 | 1 | 9 | 115 | 112 | 1 | -5 | 6 | 9 | 133 | 138 | 1 | 5 | 10 | 9 | 47 | 46 | 1 |
| 1 | 7 | 8 | 69 | 65 | 1 | -10 | 12 | 8 | 0 | 6 | 1 | 7 | 1 | 9 | 0 | 14 | 1 | -4 | 6 | 9 | 120 | 122 | 1 | 6 | 10 | 9 | 85 | 74 | 1 |
| 2 | 7 | 8 | 16 | 3 | 4 | -9 | 12 | 8 | 33 | 32 | 1 | 8 | 1 | 9 | 17 | 14 | 4 | -3 | 6 | 9 | 114 | 112 | 1 | 7 | 10 | 9 | 39 | 39 | 1 |
| 3 | 7 | 8 | 116 | 116 | 1 | -8 | 12 | 8 | 40 | 37 | 9 | -11 | 2 | 9 | 0 | 2 | 1 | -2 | 6 | 9 | 232 | 235 | 1 | -10 | 11 | 9 | 57 | 52 | 1 |
| 4 | 7 | 8 | 100 | 102 | 1 | -7 | 12 | 8 | 9 | 7 | 2 | -10 | 2 | 9 | 54 | 52 | 1 | -1 | 6 | 9 | 148 | 133 | 1 | -9 | 11 | 9 | 25 | 24 | 1 |
| 5 | 7 | 8 | 34 | 36 | 1 | -6 | 12 | 8 | 14 | 14 | 1 | -9 | 2 | 9 | 176 | 190 | 11 | 0 | 6 | 9 | 36 | 38 | 1 | -8 | 11 | 9 | 66 | 60 | 2 |
| 6 | 7 | 8 | 39 | 36 | 1 | -5 | 12 | 8 | 22 | 24 | 1 | -8 | 2 | 9 | 168 | 172 | 2 | 1 | 6 | 9 | 64 | 64 | 1 | -7 | 11 | 9 | 59 | 52 | 1 |
| 8 | 7 | 8 | 13 | 7 | 4 | -4 | 12 | 8 | 102 | 103 | 4 | -7 | 2 | 9 | 94 | 93 | 4 | 2 | 6 | 9 | 84 | 87 | 1 | -6 | 11 | 9 | 65 | 67 | 1 |
| -12 | 8 | 8 | 20 | 29 | 2 | -3 | 12 | 8 | 42 | 44 | 1 | -6 | 2 | 9 | 108 | 107 | 1 | 3 | 6 | 9 | 9 | 13 | 3 | -5 | 11 | 9 | 29 | 29 | 1 |
| -11 | 8 | 8 | 33 | 31 | 1 | -2 | 12 | 8 | 42 | 44 | 1 | -5 | 2 | 9 | 217 | 222 | 1 | 4 | 6 | 9 | 40 | 47 | 1 | -4 | 11 | 9 | 62 | 62 | 1 |
| -10 | 8 | 8 | 9 | 7 | 5 | -1 | 12 | 8 | 53 | 51 | 1 | -4 | 2 | 9 | 114 | 116 | 1 | 5 | 6 | 9 | 42 | 38 | 3 | -3 | 11 | 9 | 13 | 16 | 1 |
| -9 | 8 | 8 | 80 | 79 | 1 | 0 | 12 | 8 | 16 | 18 | 1 | -3 | 2 | 9 | 14 | 4 | 6 | 7 | 6 | 9 | 18 | 11 | 2 | -2 | 11 | 9 | 61 | 58 | 1 |
| -8 | 8 | 8 | 33 | 35 | 2 | 1 | 12 | 8 | 34 | 30 | 1 | -2 | 2 | 9 | 28 | 23 | 1 | 8 | 6 | 9 | 0 | 0 | 1 | -1 | 11 | 9 | 42 | 44 | 1 |
| -7 | 8 | 8 | 15 | 16 | 1 | 2 | 12 | 8 | 13 | 15 | 1 | -1 | 2 | 9 | 403 | 395 | 2 | 9 | 6 | 9 | 28 | 26 | 3 | 0 | 11 | 9 | 80 | 82 | 1 |
| -6 | 8 | 8 | 91 | 94 | 2 | 3 | 12 | 8 | 14 | 16 | 2 | 0 | 2 | 9 | 233 | 246 | 2 | -11 | 7 | 9 | 20 | 14 | 2 | 1 | 11 | 9 | 43 | 44 | 1 |
| -5 | 8 | 8 | 146 | 142 | 1 | 4 | 12 | 8 | 55 | 58 | 1 | 1 | 2 | 9 | 88 | 94 | 1 | -9 | 7 | 9 | 12 | 6 | 2 | 2 | 11 | 9 | 52 | 58 | 2 |
| -4 | 8 | 8 | 137 | 135 | 2 | 5 | 12 | 8 | 28 | 28 | 2 | 2 | 2 | 9 | 21 | 17 | 1 | -8 | 7 | 9 | 65 | 67 | 1 | 3 | 11 | 9 | 44 | 45 | 1 |
| -3 | 8 | 8 | 16 | 20 | 2 | 6 | 12 | 8 | 9 | 5 | 3 | 3 | 2 | 9 | 7 | 12 | 4 | -7 | 7 | 9 | 27 | 23 | 1 | 4 | 11 | 9 | 13 | 15 | 2 |
| -2 | 8 | 8 | 11 | 17 | 2 | 7 | 12 | 8 | 11 | 11 | 3 | 4 | 2 | 9 | 215 | 219 | 1 | -6 | 7 | 9 | 128 | 127 | 1 | 5 | 11 | 9 | 16 | 8 | 2 |
| -1 | 8 | 8 | 49 | 52 | 1 | -7 | 13 | 8 | 27 | 24 | 1 | 5 | 2 | 9 | 88 | 85 | 1 | -5 | 7 | 9 | 113 | 114 | 1 | -11 | 12 | 9 | 11 | 8 | 4 |
| 0 | 8 | 8 | 77 | 83 | 1 | -6 | 13 | 8 | 25 | 22 | 2 | 6 | 2 | 9 | 56 | 57 | 2 | -4 | 7 | 9 | 187 | 189 | 1 | -10 | 12 | 9 | 14 | 16 | 2 |
| 1 | 8 | 8 | 14 | 18 | 1 | -5 | 13 | 8 | 8 | 4 | 2 | 7 | 2 | 9 | 80 | 78 | 1 | -3 | 7 | 9 | 43 | 41 | 1 | -9 | 12 | 9 | 27 | 26 | 1 |
| 2 | 8 | 8 | 185 | 179 | 1 | -4 | 13 | 8 | 24 | 31 | 1 | -11 | 3 | 9 | 13 | 9 | 3 | -2 | 7 | 9 | 88 | 90 | 1 | -8 | 12 | 9 | 28 | 25 | 1 |
| 3 | 8 | 8 | 12 | 3 | 5 | -3 | 13 | 8 | 81 | 76 | 1 | -10 | 3 | 9 | 50 | 62 | 1 | -1 | 7 | 9 | 154 | 153 | 1 | -7 | 12 | 9 | 38 | 36 | 1 |
| 4 | 8 | 8 | 15 | 16 | 2 | -2 | 13 | 8 | 44 | 47 | 1 | -9 | 3 | 9 | 122 | 120 | 1 | 0 | 7 | 9 | 0 | 5 | 1 | -6 | 12 | 9 | 0 | 5 | 1 |
| 5 | 8 | 8 | 12 | 14 | 2 | -1 | 13 | 8 | 66 | 68 | 1 | -8 | 3 | 9 | 128 | 126 | 1 | 1 | 7 | 9 | 41 | 44 | 1 | -5 | 12 | 9 | 7 | 3 | 4 |
| 6 | 8 | 8 | 9 | 1 | 4 | 0 | 13 | 8 | 9 | 3 | 2 | -7 | 3 | 9 | 82 | 85 | 1 | 2 | 7 | 9 | 99 | 93 | 1 | -4 | 12 | 9 | 22 | 26 | 1 |
| 7 | 8 | 8 | 49 | 50 | 1 | 1 | 13 | 8 | 27 | 27 | 1 | -6 | 3 | 9 | 79 | 77 | 1 | 3 | 7 | 9 | 334 | 327 | 2 | -3 | 12 | 9 | 35 | 33 | 1 |
| 8 | 8 | 8 | 19 | 19 | 3 | 2 | 13 | 8 | 28 | 28 | 5 | -5 | 3 | 9 | 41 | 43 | 1 | 4 | 7 | 9 | 61 | 54 | 1 | -2 | 12 | 9 | 38 | 33 | 2 |
| 9 | 8 | 8 | 23 | 22 | 2 | 3 | 13 | 8 | 24 | 26 | 9 | -4 | 3 | 9 | 121 | 119 | 1 | 5 | 7 | 9 | 47 | 44 | 1 | -1 | 12 | 9 | 154 | 145 | 2 |
| -10 | 9 | 8 | 12 | 6 | 4 | 5 | 13 | 8 | 0 | 2 | 1 | -3 | 3 | 9 | 82 | 89 | 2 | 6 | 7 | 9 | 9 | 1 | 9 | 0 | 12 | 9 | 28 | 29 | 1 |
| -9 | 9 | 8 | 26 | 26 | 3 | 7 | 13 | 8 | 0 | 0 | 1 | -2 | 3 | 9 | 58 | 53 | 1 | 7 | 7 | 9 | 0 | 1 | 1 | 1 | 12 | 9 | 6 | 8 | 5 |
| -8 | 9 | 8 | 48 | 43 | 1 | -6 | 14 | 8 | 30 | 36 | 2 | -1 | 3 | 9 | 372 | 358 | 2 | 8 | 7 | 9 | 9 | 16 | 9 | 2 | 12 | 9 | 50 | 42 | 3 |
| -7 | 9 | 8 | 91 | 90 | 1 | -4 | 14 | 8 | 26 | 36 | 26 | 0 | 3 | 9 | 265 | 265 | 3 | -12 | 8 | 9 | 67 | 55 | 1 | 3 | 12 | 9 | 71 | 65 | 1 |
| -6 | 9 | 8 | 35 | 38 | 1 | -3 | 14 | 8 | 8 | 15 | 2 | 1 | 3 | 9 | 32 | 34 | 1 | -11 | 8 | 9 | 0 | 10 | 1 | 4 | 12 | 9 | 11 | 6 | 2 |
| -5 | 9 | 8 | 126 | 121 | 1 | -2 | 14 | | | | | | | | | | | | | | | | | | | | | | |

Table 10. Observed and calculated structure factors for pchm26

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|-----|----|----|------|------|-----|-----|---|----|------|------|-----|-----|----|----|------|------|-----|-----|----|----|------|------|-----|-----|---|----|------|------|-----|
| -5 | 15 | 9 | 111 | 97 | 1 | -5 | 3 | 10 | 225 | 234 | 1 | 3 | 7 | 10 | 84 | 75 | 1 | -3 | 12 | 10 | 42 | 41 | 1 | -10 | 2 | 11 | 0 | 11 | 1 |
| -4 | 15 | 9 | 0 | 12 | 1 | -4 | 3 | 10 | 87 | 88 | 1 | 4 | 7 | 10 | 26 | 31 | 1 | -2 | 12 | 10 | 84 | 79 | 2 | -9 | 2 | 11 | 0 | 10 | 1 |
| -3 | 15 | 9 | 69 | 61 | 1 | -3 | 3 | 10 | 86 | 89 | 1 | 5 | 7 | 10 | 18 | 19 | 1 | -1 | 12 | 10 | 9 | 1 | 3 | -8 | 2 | 11 | 113 | 113 | 1 |
| -2 | 15 | 9 | 40 | 45 | 1 | -2 | 3 | 10 | 143 | 143 | 1 | 6 | 7 | 10 | 16 | 15 | 2 | 0 | 12 | 10 | 39 | 39 | 1 | -7 | 2 | 11 | 129 | 135 | 1 |
| -1 | 15 | 9 | 18 | 20 | 1 | -1 | 3 | 10 | 198 | 198 | 2 | 7 | 7 | 10 | 11 | 13 | 7 | 1 | 12 | 10 | 20 | 20 | 1 | -6 | 2 | 11 | 11 | 12 | 2 |
| 0 | 15 | 9 | 11 | 2 | 2 | 0 | 3 | 10 | 114 | 115 | 1 | 8 | 7 | 10 | 25 | 29 | 2 | 2 | 12 | 10 | 36 | 34 | 1 | -5 | 2 | 11 | 9 | 18 | 2 |
| 1 | 15 | 9 | 13 | 13 | 1 | 1 | 3 | 10 | 54 | 55 | 1 | -12 | 8 | 10 | 27 | 19 | 1 | 3 | 12 | 10 | 45 | 52 | 1 | -4 | 2 | 11 | 118 | 122 | 1 |
| 2 | 15 | 9 | 59 | 57 | 1 | 2 | 3 | 10 | 111 | 110 | 1 | -11 | 8 | 10 | 22 | 23 | 2 | 4 | 12 | 10 | 17 | 14 | 1 | -3 | 2 | 11 | 41 | 42 | 1 |
| -7 | 16 | 9 | 0 | 11 | 1 | 3 | 3 | 10 | 97 | 105 | 1 | -8 | 8 | 10 | 62 | 59 | 1 | 5 | 12 | 10 | 19 | 18 | 4 | -2 | 2 | 11 | 131 | 127 | 1 |
| -4 | 16 | 9 | 66 | 63 | 1 | 4 | 3 | 10 | 54 | 56 | 1 | -7 | 8 | 10 | 54 | 50 | 1 | -10 | 13 | 10 | 11 | 4 | 2 | -1 | 2 | 11 | 56 | 65 | 2 |
| -3 | 16 | 9 | 0 | 6 | 1 | 5 | 3 | 10 | 52 | 56 | 3 | -6 | 8 | 10 | 84 | 80 | 1 | -9 | 13 | 10 | 15 | 17 | 4 | 0 | 2 | 11 | 169 | 170 | 1 |
| -2 | 16 | 9 | 65 | 75 | 16 | 6 | 3 | 10 | 78 | 68 | 1 | -5 | 8 | 10 | 0 | 10 | 1 | -8 | 13 | 10 | 26 | 29 | 1 | 1 | 2 | 11 | 120 | 123 | 1 |
| -1 | 16 | 9 | 81 | 86 | 1 | 7 | 3 | 10 | 20 | 22 | 4 | -4 | 8 | 10 | 18 | 27 | 6 | -7 | 13 | 10 | 8 | 3 | 3 | 2 | 2 | 11 | 216 | 218 | 1 |
| 0 | 16 | 9 | 0 | 5 | 1 | 8 | 3 | 10 | 40 | 46 | 2 | -3 | 8 | 10 | 10 | 5 | 2 | -6 | 13 | 10 | 29 | 34 | 1 | 3 | 2 | 11 | 12 | 10 | 2 |
| 1 | 16 | 9 | 41 | 39 | 1 | -11 | 4 | 10 | 21 | 24 | 2 | -2 | 8 | 10 | 136 | 137 | 3 | -5 | 13 | 10 | 64 | 61 | 1 | 4 | 2 | 11 | 7 | 2 | 7 |
| 3 | 16 | 9 | 0 | 5 | 1 | -9 | 4 | 10 | 55 | 52 | 1 | -1 | 8 | 10 | 98 | 100 | 2 | -4 | 13 | 10 | 43 | 43 | 1 | 5 | 2 | 11 | 77 | 72 | 1 |
| 4 | 16 | 9 | 0 | 8 | 1 | -8 | 4 | 10 | 44 | 53 | 1 | 0 | 8 | 10 | 50 | 47 | 1 | -3 | 13 | 10 | 28 | 28 | 1 | 6 | 2 | 11 | 29 | 30 | 1 |
| -5 | 17 | 9 | 13 | 16 | 7 | -7 | 4 | 10 | 89 | 84 | 1 | 1 | 8 | 10 | 92 | 91 | 1 | -2 | 13 | 10 | 56 | 53 | 2 | 7 | 2 | 11 | 44 | 40 | 1 |
| -4 | 17 | 9 | 18 | 17 | 2 | -6 | 4 | 10 | 152 | 157 | 1 | 2 | 8 | 10 | 15 | 17 | 1 | -1 | 13 | 10 | 16 | 17 | 1 | 8 | 2 | 11 | 22 | 15 | 3 |
| -3 | 17 | 9 | 44 | 44 | 1 | -5 | 4 | 10 | 76 | 81 | 1 | 3 | 8 | 10 | 12 | 15 | 2 | 0 | 13 | 10 | 18 | 16 | 1 | -11 | 3 | 11 | 18 | 9 | 2 |
| -2 | 17 | 9 | 22 | 27 | 8 | -4 | 4 | 10 | 161 | 161 | 2 | 4 | 8 | 10 | 0 | 9 | 1 | 1 | 13 | 10 | 16 | 19 | 1 | -10 | 3 | 11 | 18 | 13 | 1 |
| -1 | 17 | 9 | 28 | 36 | 2 | -3 | 4 | 10 | 140 | 147 | 1 | 5 | 8 | 10 | 29 | 28 | 1 | 3 | 13 | 10 | 14 | 19 | 4 | -9 | 3 | 11 | 20 | 27 | 1 |
| 1 | 17 | 9 | 9 | 3 | 9 | -2 | 4 | 10 | 33 | 33 | 1 | 6 | 8 | 10 | 143 | 133 | 1 | 4 | 13 | 10 | 13 | 27 | 2 | -8 | 3 | 11 | 9 | 10 | 5 |
| 2 | 17 | 9 | 37 | 40 | 1 | -1 | 4 | 10 | 127 | 126 | 1 | 7 | 8 | 10 | 0 | 8 | 1 | 5 | 13 | 10 | 15 | 27 | 4 | -7 | 3 | 11 | 38 | 36 | 1 |
| -4 | 18 | 9 | 10 | 12 | 6 | 0 | 4 | 10 | 87 | 83 | 1 | 8 | 8 | 10 | 0 | 7 | 1 | 6 | 13 | 10 | 19 | 21 | 1 | -6 | 3 | 11 | 51 | 48 | 1 |
| -3 | 18 | 9 | 14 | 6 | 2 | 1 | 4 | 10 | 32 | 36 | 1 | -12 | 9 | 10 | 19 | 25 | 4 | -6 | 14 | 10 | 8 | 11 | 4 | -5 | 3 | 11 | 58 | 65 | 1 |
| -2 | 18 | 9 | 9 | 10 | 5 | 2 | 4 | 10 | 57 | 57 | 1 | -11 | 9 | 10 | 22 | 29 | 1 | -5 | 14 | 10 | 9 | 10 | 9 | -4 | 3 | 11 | 42 | 40 | 3 |
| 0 | 18 | 9 | 13 | 24 | 4 | 3 | 4 | 10 | 15 | 17 | 1 | -10 | 9 | 10 | 37 | 33 | 1 | -4 | 14 | 10 | 19 | 21 | 1 | -3 | 3 | 11 | 29 | 28 | 1 |
| -9 | 0 | 10 | 70 | 78 | 1 | 4 | 4 | 10 | 99 | 103 | 1 | -9 | 9 | 10 | 30 | 32 | 1 | -3 | 14 | 10 | 11 | 0 | 2 | -2 | 3 | 11 | 102 | 102 | 1 |
| -8 | 0 | 10 | 12 | 7 | 3 | 5 | 4 | 10 | 124 | 118 | 4 | -8 | 9 | 10 | 69 | 64 | 1 | -2 | 14 | 10 | 32 | 34 | 1 | -1 | 3 | 11 | 25 | 28 | 1 |
| -7 | 0 | 10 | 166 | 166 | 1 | 6 | 4 | 10 | 65 | 70 | 1 | -7 | 9 | 10 | 81 | 74 | 1 | -1 | 14 | 10 | 50 | 50 | 1 | 0 | 3 | 11 | 55 | 58 | 1 |
| -6 | 0 | 10 | 101 | 104 | 1 | 9 | 4 | 10 | 37 | 31 | 2 | -5 | 9 | 10 | 65 | 67 | 1 | 1 | 14 | 10 | 13 | 8 | 2 | 2 | 3 | 11 | 15 | 18 | 1 |
| -5 | 0 | 10 | 590 | 593 | 5 | -12 | 5 | 10 | 0 | 9 | 1 | -4 | 9 | 10 | 13 | 15 | 1 | 2 | 14 | 10 | 73 | 78 | 17 | 3 | 3 | 11 | 75 | 80 | 1 |
| -4 | 0 | 10 | 77 | 85 | 1 | -11 | 5 | 10 | 26 | 26 | 1 | -3 | 9 | 10 | 117 | 105 | 1 | 5 | 14 | 10 | 12 | 15 | 3 | 4 | 3 | 11 | 14 | 18 | 1 |
| -3 | 0 | 10 | 30 | 28 | 1 | -10 | 5 | 10 | 52 | 45 | 1 | -2 | 9 | 10 | 81 | 76 | 1 | -7 | 15 | 10 | 0 | 0 | 1 | 5 | 3 | 11 | 83 | 79 | 3 |
| -2 | 0 | 10 | 258 | 257 | 2 | -9 | 5 | 10 | 57 | 59 | 7 | -1 | 9 | 10 | 93 | 104 | 1 | -6 | 15 | 10 | 32 | 34 | 1 | 6 | 3 | 11 | 84 | 82 | 1 |
| -1 | 0 | 10 | 118 | 117 | 1 | -8 | 5 | 10 | 114 | 108 | 2 | 0 | 9 | 10 | 85 | 84 | 2 | -5 | 15 | 10 | 17 | 17 | 2 | 7 | 3 | 11 | 19 | 24 | 4 |
| 0 | 0 | 10 | 25 | 24 | 1 | -7 | 5 | 10 | 54 | 56 | 1 | 1 | 9 | 10 | 47 | 50 | 1 | -4 | 15 | 10 | 0 | 0 | 1 | -12 | 4 | 11 | 51 | 48 | 1 |
| 2 | 0 | 10 | 407 | 412 | 3 | -6 | 5 | 10 | 150 | 148 | 1 | 2 | 9 | 10 | 25 | 28 | 2 | -3 | 15 | 10 | 0 | 6 | 1 | -10 | 4 | 11 | 9 | 4 | 7 |
| 3 | 0 | 10 | 209 | 209 | 1 | -5 | 5 | 10 | 206 | 209 | 1 | 4 | 9 | 10 | 31 | 32 | 3 | -2 | 15 | 10 | 14 | 9 | 1 | -9 | 4 | 11 | 121 | 120 | 1 |
| 4 | 0 | 10 | 277 | 279 | 2 | -4 | 5 | 10 | 58 | 57 | 1 | 5 | 9 | 10 | 12 | 8 | 2 | -1 | 15 | 10 | 11 | 17 | 2 | -8 | 4 | 11 | 52 | 57 | 1 |
| 5 | 0 | 10 | 40 | 43 | 1 | -3 | 5 | 10 | 39 | 38 | 1 | 6 | 9 | 10 | 23 | 18 | 1 | 0 | 15 | 10 | 12 | 3 | 8 | -7 | 4 | 11 | 56 | 69 | 1 |
| 6 | 0 | 10 | 75 | 73 | 1 | -2 | 5 | 10 | 150 | 150 | 1 | 7 | 9 | 10 | 8 | 4 | 8 | 1 | 15 | 10 | 7 | 7 | 6 | -6 | 4 | 11 | 69 | 63 | 1 |
| 7 | 0 | 10 | 13 | 9 | 6 | -1 | 5 | 10 | 80 | 79 | 1 | 8 | 9 | 10 | 0 | 16 | 1 | 2 | 15 | 10 | 16 | 20 | 15 | -5 | 4 | 11 | 91 | 90 | 1 |
| -12 | 1 | 10 | 19 | 4 | 2 | 0 | 5 | 10 | 48 | 50 | 1 | -11 | 10 | 10 | 0 | 3 | 1 | 3 | 15 | 10 | 42 | 38 | 1 | -4 | 4 | 11 | 0 | 8 | 1 |
| -11 | 1 | 10 | 21 | 26 | 2 | 1 | 5 | 10 | 38 | 41 | 1 | -10 | 10 | 10 | 8 | 10 | 7 | -7 | 16 | 10 | 15 | 5 | 8 | -3 | 4 | 11 | 55 | 52 | 1 |
| -9 | 1 | 10 | 10 | 2 | 2 | 2 | 5 | 10 | 15 | 10 | 1 | -9 | 10 | 10 | 15 | 14 | 1 | -6 | 16 | 10 | 14 | 6 | 3 | -2 | 4 | 11 | 172 | 164 | 1 |
| -8 | 1 | 10 | 56 | 55 | 1 | 3 | 5 | 10 | 51 | 53 | 1 | -8 | 10 | 10 | 37 | 32 | 1 | -5 | 16 | 10 | 16 | 21 | 3 | -1 | 4 | 11 | 187 | 181 | 1 |
| -7 | 1 | 10 | 12 | 16 | 1 | 4 | 5 | 10 | 123 | 122 | 1 | -7 | 10 | 10 | 13 | 13 | 1 | -4 | 16 | 10 | 5 | 12 | 5 | 0 | 4 | 11 | 27 | 26 | 4 |
| -6 | 1 | 10 | 139 | 146 | 2 | 5 | 5 | 10 | 49 | 43 | 1 | -6 | 10 | 10 | 46 | 47 | 1 | -3 | 16 | 10 | 19 | 17 | 5 | 1 | 4 | 11 | 79 | 81 | 2 |
| -5 | 1 | 10 | 89 | 83 | 1 | 7 | 5 | 10 | 0 | 12 | 1 | -5 | 10 | 10 | 91 | 90 | 1 | -2 | 16 | 10 | 10 | 10 | 2 | 2 | 4 | 11 | 19 | 14 | 1 |
| -4 | 1 | 10 | 56 | 55 | 2 | 8 | 5 | 10 | 0 | 5 | 1 | -4 | 10 | 10 | 76 | 73 | 1 | -1 | 16 | 10 | 11 | 8 | 2 | 3 | 4 | 11 | 21 | 28 | 1 |
| -3 | 1 | 10 | 82 | 85 | 1 | -11 | 6 | 10 | 21 | 17 | 2 | -3 | 10 | 10 | 51 | 49 | 1 | 0 | 16 | 10 | 0 | 6 | 1 | 4 | 4 | 11 | 95 | 97 | 2 |
| -2 | 1 | 10 | 183 | 184 | 1 | -9 | 6 | 10 | 11 | 4 | 4 | -2 | 10 | 10 | 10 | 11 | 2 | 1 | 16 | 10 | 22 | 30 | 11 | 5 | 4 | 11 | 23 | 29 | 1 |
| -1 | 1 | 10 | 244 | 249 | 2 | -8 | 6 | 10 | 27 | 31 | 1 | -1 | 10 | 10 | 110 | 117 | 1 | 3 | 16 | 10 | 0 | 8 | 1 | 6 | 4 | 11 | 74 | 79 | 8 |
| 0 | 1 | 10 | 136 | 139 | 1 | -7 | 6 | 10 | 124 | 124 | 3 | 0 | 10 | 10 | 32 | 34 | 1 | -5 | 17 | 10 | 0 | 13 | 1 | 7 | 4 | 11 | 35 | 36 | 2 |
| 1 | 1 | 10 | 98 | 108 | 1 | -6 | 6 | 10 | 65 | 68 | 1 | 1 | 10 | 10 | 12 | 15 | 1 | -4 | 17 | 10 | 0 | 5 | 1 | 8 | 4 | 11 | 36 | 40 | 1 |
| 2 | 1 | 10 | 190 | 189 | 1 | -5 | 6 | 10 | 132 | 142 | 1 | 2 | 10 | 10 | 15 | 26 | 2 | -3 | 17 | 10 | 9 | 11 | 8 | -12 | 5 | 11 | 43 | 40 | 1 |
| 3 | 1 | 10 | 248 | 252 | 1 | -4 | 6 | 10 | 35 | 39 | 2 | 3 | 10 | 10 | 16 | 22 | 1 | -2 | 17 | 10 | 27 | 28 | 1 | -11 | 5 | 11 | 31 | 28 | 1 |
| 4 | 1 | 10 | 97 | 93 | 1 | -3 | 6 | 10 | 23 | | | | | | | | | | | | | | | | | | | | |

Table 10.

Observed and calculated structure factors for pchm26

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|-----|---|----|------|------|-----|-----|----|----|------|------|-----|-----|---|----|------|------|-----|-----|---|----|------|------|-----|-----|----|----|------|------|-----|
| -2 | 6 | 11 | 64 | 71 | 1 | -9 | 11 | 11 | 45 | 38 | 1 | -11 | 0 | 12 | 12 | 16 | 7 | 3 | 4 | 12 | 74 | 76 | 1 | -9 | 9 | 12 | 12 | 7 | 2 |
| -1 | 6 | 11 | 13 | 17 | 5 | -8 | 11 | 11 | 15 | 25 | 1 | -9 | 0 | 12 | 69 | 70 | 1 | 4 | 4 | 12 | 86 | 85 | 1 | -8 | 9 | 12 | 42 | 41 | 1 |
| 0 | 6 | 11 | 15 | 22 | 1 | -7 | 11 | 11 | 27 | 29 | 1 | -8 | 0 | 12 | 123 | 118 | 1 | 5 | 4 | 12 | 48 | 48 | 1 | -7 | 9 | 12 | 48 | 47 | 1 |
| 1 | 6 | 11 | 17 | 17 | 1 | -6 | 11 | 11 | 15 | 27 | 1 | -7 | 0 | 12 | 200 | 210 | 1 | 6 | 4 | 12 | 33 | 41 | 1 | -6 | 9 | 12 | 6 | 2 | 6 |
| 2 | 6 | 11 | 49 | 51 | 2 | -5 | 11 | 11 | 30 | 29 | 1 | -6 | 0 | 12 | 19 | 25 | 1 | 7 | 4 | 12 | 27 | 41 | 3 | -5 | 9 | 12 | 22 | 24 | 1 |
| 3 | 6 | 11 | 11 | 9 | 5 | -4 | 11 | 11 | 7 | 5 | 2 | -5 | 0 | 12 | 263 | 265 | 2 | 8 | 4 | 12 | 24 | 27 | 3 | -4 | 9 | 12 | 77 | 78 | 1 |
| 4 | 6 | 11 | 15 | 24 | 2 | -3 | 11 | 11 | 13 | 1 | 1 | -4 | 0 | 12 | 176 | 169 | 1 | -12 | 5 | 12 | 10 | 5 | 10 | -3 | 9 | 12 | 137 | 134 | 2 |
| 5 | 6 | 11 | 80 | 68 | 3 | -2 | 11 | 11 | 46 | 51 | 1 | -3 | 0 | 12 | 73 | 79 | 1 | -11 | 5 | 12 | 0 | 5 | 1 | -2 | 9 | 12 | 51 | 57 | 1 |
| 6 | 6 | 11 | 44 | 50 | 1 | -1 | 11 | 11 | 8 | 0 | 5 | -2 | 0 | 12 | 73 | 71 | 1 | -10 | 5 | 12 | 18 | 20 | 2 | -1 | 9 | 12 | 57 | 59 | 1 |
| 7 | 6 | 11 | 13 | 7 | 5 | 0 | 11 | 11 | 36 | 35 | 1 | -1 | 0 | 12 | 66 | 76 | 1 | -9 | 5 | 12 | 109 | 107 | 1 | 0 | 9 | 12 | 28 | 31 | 1 |
| -12 | 7 | 11 | 48 | 42 | 1 | 1 | 11 | 11 | 11 | 8 | 2 | 0 | 0 | 12 | 144 | 134 | 1 | -8 | 5 | 12 | 123 | 120 | 1 | 1 | 9 | 12 | 42 | 40 | 2 |
| -11 | 7 | 11 | 18 | 2 | 3 | 2 | 11 | 11 | 15 | 15 | 1 | 1 | 0 | 12 | 39 | 41 | 1 | -7 | 5 | 12 | 12 | 5 | 8 | 2 | 9 | 12 | 88 | 88 | 1 |
| -10 | 7 | 11 | 15 | 14 | 2 | 3 | 11 | 11 | 15 | 17 | 1 | 2 | 0 | 12 | 227 | 227 | 2 | -6 | 5 | 12 | 132 | 132 | 1 | 3 | 9 | 12 | 0 | 1 | 1 |
| -9 | 7 | 11 | 32 | 34 | 4 | 4 | 11 | 11 | 12 | 6 | 4 | 3 | 0 | 12 | 102 | 98 | 1 | -5 | 5 | 12 | 72 | 74 | 1 | 4 | 9 | 12 | 24 | 21 | 1 |
| -8 | 7 | 11 | 151 | 139 | 1 | 6 | 11 | 11 | 12 | 14 | 3 | 4 | 0 | 12 | 73 | 69 | 1 | -4 | 5 | 12 | 221 | 219 | 2 | 5 | 9 | 12 | 16 | 8 | 6 |
| -7 | 7 | 11 | 27 | 23 | 3 | -10 | 12 | 11 | 0 | 0 | 1 | 5 | 0 | 12 | 27 | 32 | 2 | -3 | 5 | 12 | 29 | 30 | 1 | 6 | 9 | 12 | 0 | 4 | 1 |
| -6 | 7 | 11 | 66 | 74 | 3 | -8 | 12 | 11 | 20 | 19 | 1 | 6 | 0 | 12 | 0 | 1 | 1 | -2 | 5 | 12 | 184 | 181 | 1 | -11 | 10 | 12 | 9 | 16 | 8 |
| -5 | 7 | 11 | 96 | 93 | 1 | -7 | 12 | 11 | 24 | 22 | 4 | -12 | 1 | 12 | 14 | 0 | 8 | -1 | 5 | 12 | 149 | 143 | 1 | -10 | 10 | 12 | 40 | 35 | 1 |
| -4 | 7 | 11 | 0 | 18 | 1 | -6 | 12 | 11 | 68 | 66 | 3 | -10 | 1 | 12 | 16 | 21 | 2 | 0 | 5 | 12 | 52 | 57 | 1 | -9 | 10 | 12 | 23 | 25 | 3 |
| -3 | 7 | 11 | 26 | 25 | 1 | -5 | 12 | 11 | 39 | 37 | 1 | -9 | 1 | 12 | 100 | 99 | 3 | 1 | 5 | 12 | 71 | 68 | 1 | -8 | 10 | 12 | 8 | 5 | 8 |
| -2 | 7 | 11 | 289 | 288 | 1 | -4 | 12 | 11 | 54 | 52 | 1 | -8 | 1 | 12 | 85 | 98 | 1 | 2 | 5 | 12 | 147 | 144 | 5 | -7 | 10 | 12 | 8 | 7 | 3 |
| -1 | 7 | 11 | 4 | 5 | 4 | -3 | 12 | 11 | 8 | 4 | 2 | -7 | 1 | 12 | 52 | 55 | 1 | 3 | 5 | 12 | 6 | 18 | 5 | -6 | 10 | 12 | 8 | 7 | 3 |
| 0 | 7 | 11 | 71 | 72 | 1 | -2 | 12 | 11 | 36 | 37 | 1 | -6 | 1 | 12 | 54 | 64 | 2 | 4 | 5 | 12 | 13 | 16 | 3 | -5 | 10 | 12 | 22 | 23 | 1 |
| 1 | 7 | 11 | 115 | 114 | 1 | -1 | 12 | 11 | 12 | 18 | 2 | -5 | 1 | 12 | 14 | 13 | 2 | 5 | 5 | 12 | 13 | 11 | 2 | -4 | 10 | 12 | 33 | 34 | 1 |
| 2 | 7 | 11 | 109 | 110 | 1 | 0 | 12 | 11 | 15 | 15 | 1 | -4 | 1 | 12 | 18 | 14 | 1 | 6 | 5 | 12 | 38 | 39 | 2 | -3 | 10 | 12 | 72 | 71 | 1 |
| 3 | 7 | 11 | 83 | 80 | 5 | 1 | 12 | 11 | 66 | 61 | 1 | -3 | 1 | 12 | 9 | 0 | 2 | 7 | 5 | 12 | 12 | 11 | 6 | -2 | 10 | 12 | 70 | 73 | 1 |
| 4 | 7 | 11 | 43 | 44 | 1 | 2 | 12 | 11 | 17 | 22 | 2 | -2 | 1 | 12 | 160 | 171 | 2 | 8 | 5 | 12 | 0 | 5 | 1 | -1 | 10 | 12 | 49 | 50 | 1 |
| 5 | 7 | 11 | 42 | 41 | 3 | 3 | 12 | 11 | 10 | 3 | 2 | -1 | 1 | 12 | 38 | 46 | 1 | -12 | 6 | 12 | 37 | 37 | 1 | 0 | 10 | 12 | 68 | 65 | 3 |
| 6 | 7 | 11 | 61 | 62 | 1 | 4 | 12 | 11 | 13 | 13 | 2 | 0 | 1 | 12 | 133 | 137 | 1 | -11 | 6 | 12 | 13 | 13 | 5 | 1 | 10 | 12 | 46 | 47 | 1 |
| 8 | 7 | 11 | 15 | 5 | 4 | 5 | 12 | 11 | 16 | 17 | 6 | 1 | 1 | 12 | 129 | 128 | 1 | -10 | 6 | 12 | 57 | 56 | 1 | 2 | 10 | 12 | 23 | 26 | 1 |
| -12 | 8 | 11 | 13 | 18 | 6 | 6 | 12 | 11 | 5 | 10 | 5 | 2 | 1 | 12 | 116 | 115 | 1 | -9 | 6 | 12 | 42 | 39 | 1 | 3 | 10 | 12 | 38 | 37 | 1 |
| -11 | 8 | 11 | 0 | 9 | 1 | -10 | 13 | 11 | 0 | 0 | 1 | 3 | 1 | 12 | 90 | 91 | 1 | -8 | 6 | 12 | 13 | 14 | 2 | 4 | 10 | 12 | 25 | 23 | 1 |
| -10 | 8 | 11 | 8 | 9 | 8 | -9 | 13 | 11 | 50 | 45 | 1 | 4 | 1 | 12 | 31 | 39 | 1 | -7 | 6 | 12 | 115 | 120 | 1 | 5 | 10 | 12 | 18 | 9 | 2 |
| -9 | 8 | 11 | 9 | 9 | 6 | -8 | 13 | 11 | 45 | 45 | 1 | 5 | 1 | 12 | 37 | 40 | 1 | -6 | 6 | 12 | 95 | 95 | 1 | 6 | 10 | 12 | 0 | 22 | 1 |
| -8 | 8 | 11 | 24 | 26 | 1 | -7 | 13 | 11 | 51 | 48 | 1 | 6 | 1 | 12 | 14 | 7 | 7 | -5 | 6 | 12 | 203 | 206 | 1 | -11 | 11 | 12 | 11 | 16 | 7 |
| -7 | 8 | 11 | 141 | 139 | 2 | -6 | 13 | 11 | 32 | 32 | 2 | -11 | 2 | 12 | 20 | 30 | 3 | -4 | 6 | 12 | 108 | 109 | 1 | -10 | 11 | 12 | 16 | 12 | 2 |
| -6 | 8 | 11 | 110 | 108 | 1 | -5 | 13 | 11 | 19 | 20 | 1 | -10 | 2 | 12 | 65 | 61 | 1 | -3 | 6 | 12 | 221 | 226 | 1 | -9 | 11 | 12 | 60 | 58 | 1 |
| -5 | 8 | 11 | 21 | 18 | 1 | -4 | 13 | 11 | 35 | 33 | 4 | -9 | 2 | 12 | 39 | 40 | 1 | -2 | 6 | 12 | 82 | 82 | 1 | -8 | 11 | 12 | 59 | 60 | 1 |
| -4 | 8 | 11 | 10 | 7 | 2 | -3 | 13 | 11 | 9 | 4 | 2 | -8 | 2 | 12 | 86 | 84 | 1 | -1 | 6 | 12 | 6 | 16 | 6 | -7 | 11 | 12 | 34 | 34 | 1 |
| -3 | 8 | 11 | 245 | 239 | 1 | -2 | 13 | 11 | 24 | 23 | 1 | -7 | 2 | 12 | 31 | 40 | 1 | 0 | 6 | 12 | 0 | 9 | 1 | -6 | 11 | 12 | 12 | 4 | 12 |
| -2 | 8 | 11 | 64 | 64 | 1 | -1 | 13 | 11 | 9 | 7 | 2 | -6 | 2 | 12 | 80 | 88 | 1 | 1 | 6 | 12 | 67 | 68 | 1 | -5 | 11 | 12 | 42 | 41 | 1 |
| -1 | 8 | 11 | 39 | 42 | 1 | 0 | 13 | 11 | 13 | 1 | 2 | -5 | 2 | 12 | 26 | 28 | 1 | 2 | 6 | 12 | 168 | 163 | 3 | -4 | 11 | 12 | 60 | 57 | 1 |
| 0 | 8 | 11 | 22 | 23 | 1 | 1 | 13 | 11 | 98 | 92 | 1 | -4 | 2 | 12 | 32 | 37 | 1 | 3 | 6 | 12 | 88 | 88 | 1 | -3 | 11 | 12 | 19 | 19 | 3 |
| 1 | 8 | 11 | 59 | 59 | 1 | 2 | 13 | 11 | 26 | 21 | 1 | -3 | 2 | 12 | 102 | 97 | 1 | 4 | 6 | 12 | 26 | 23 | 1 | -2 | 11 | 12 | 54 | 48 | 3 |
| 2 | 8 | 11 | 28 | 32 | 1 | 4 | 13 | 11 | 16 | 2 | 3 | -2 | 2 | 12 | 16 | 19 | 2 | 5 | 6 | 12 | 95 | 90 | 2 | -1 | 11 | 12 | 79 | 78 | 1 |
| 3 | 8 | 11 | 38 | 42 | 1 | 5 | 13 | 11 | 18 | 13 | 1 | -1 | 2 | 12 | 132 | 134 | 1 | 6 | 6 | 12 | 28 | 26 | 2 | 0 | 11 | 12 | 65 | 63 | 1 |
| 4 | 8 | 11 | 10 | 11 | 3 | -8 | 14 | 11 | 23 | 28 | 2 | 0 | 2 | 12 | 155 | 155 | 1 | 7 | 6 | 12 | 0 | 8 | 1 | 1 | 11 | 12 | 83 | 78 | 1 |
| 5 | 8 | 11 | 33 | 32 | 3 | -7 | 14 | 11 | 38 | 44 | 5 | 1 | 2 | 12 | 13 | 12 | 1 | -12 | 7 | 12 | 44 | 40 | 1 | 2 | 11 | 12 | 14 | 1 | 6 |
| 6 | 8 | 11 | 36 | 34 | 1 | -6 | 14 | 11 | 45 | 44 | 1 | 2 | 2 | 12 | 108 | 106 | 1 | -11 | 7 | 12 | 28 | 30 | 2 | 3 | 11 | 12 | 26 | 27 | 1 |
| -11 | 9 | 11 | 0 | 15 | 1 | -5 | 14 | 11 | 14 | 9 | 1 | 3 | 2 | 12 | 60 | 65 | 1 | -10 | 7 | 12 | 0 | 2 | 1 | 4 | 11 | 12 | 18 | 18 | 2 |
| -10 | 9 | 11 | 49 | 44 | 1 | -4 | 14 | 11 | 12 | 6 | 1 | 5 | 2 | 12 | 31 | 45 | 1 | -9 | 7 | 12 | 51 | 48 | 1 | 5 | 11 | 12 | 12 | 12 | 5 |
| -9 | 9 | 11 | 13 | 3 | 2 | -3 | 14 | 11 | 11 | 15 | 2 | 6 | 2 | 12 | 65 | 59 | 1 | -8 | 7 | 12 | 13 | 16 | 3 | -10 | 12 | 12 | 16 | 1 | 3 |
| -8 | 9 | 11 | 9 | 3 | 5 | -2 | 14 | 11 | 35 | 35 | 1 | 8 | 2 | 12 | 18 | 26 | 4 | -7 | 7 | 12 | 11 | 20 | 3 | -9 | 12 | 12 | 0 | 4 | 1 |
| -7 | 9 | 11 | 9 | 5 | 8 | -1 | 14 | 11 | 30 | 29 | 1 | -11 | 3 | 12 | 0 | 11 | 1 | -6 | 7 | 12 | 76 | 76 | 1 | -8 | 12 | 12 | 0 | 5 | 1 |
| -6 | 9 | 11 | 124 | 124 | 1 | 0 | 14 | 11 | 12 | 11 | 2 | -10 | 3 | 12 | 12 | 13 | 4 | -5 | 7 | 12 | 157 | 158 | 1 | -7 | 12 | 12 | 22 | 19 | 4 |
| -5 | 9 | 11 | 12 | 15 | 2 | 1 | 14 | 11 | 20 | 21 | 1 | -9 | 3 | 12 | 117 | 114 | 1 | -4 | 7 | 12 | 132 | 130 | 1 | -6 | 12 | 12 | 22 | 24 | 2 |
| -4 | 9 | 11 | 30 | 29 | 1 | 2 | 14 | 11 | 51 | 62 | 1 | -8 | 3 | 12 | 91 | 91 | 1 | -3 | 7 | 12 | 56 | 59 | 2 | -5 | 12 | 12 | 34 | 30 | 1 |
| -3 | 9 | 11 | 131 | 130 | 1 | 3 | 14 | 11 | 9 | 9 | 8 | -7 | 3 | 12 | 63 | 67 | 1 | -2 | 7 | 12 | 241 | 243 | 1 | -4 | 12 | 12 | 15 | 18 | 2 |
| -2 | 9 | 11 | 74 | 74 | 2 | 4 | 14 | 11 | 10 | 12 | 5 | -6 | 3 | 12 | 63 | 64 | 1 | -1 | 7 | 12 | 12 | 8 | 2 | -3 | 12 | 12 | 11 | 1 | 2 |
| -1 | 9 | 11 | 74 | | | | | | | | | | | | | | | | | | | | | | | | | | |

Table 10.

Observed and calculated structure factors for pchm26

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| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|-----|----|----|------|------|-----|-----|---|----|------|------|-----|-----|----|----|------|------|-----|-----|----|----|------|------|-----|-----|---|----|------|------|-----|
| -3 | 14 | 12 | 23 | 23 | 1 | -5 | 4 | 13 | 116 | 118 | 1 | 2 | 8 | 13 | 13 | 7 | 2 | -2 | 14 | 13 | 16 | 13 | 1 | 1 | 3 | 14 | 44 | 51 | 1 |
| -2 | 14 | 12 | 9 | 0 | 7 | -4 | 4 | 13 | 65 | 66 | 1 | 3 | 8 | 13 | 18 | 24 | 1 | -1 | 14 | 13 | 11 | 3 | 3 | 2 | 3 | 14 | 97 | 95 | 1 |
| -1 | 14 | 12 | 14 | 7 | 3 | -3 | 4 | 13 | 41 | 39 | 2 | 4 | 8 | 13 | 16 | 6 | 2 | 0 | 14 | 13 | 66 | 65 | 1 | 3 | 3 | 14 | 56 | 55 | 1 |
| 0 | 14 | 12 | 75 | 70 | 1 | -2 | 4 | 13 | 255 | 252 | 1 | 5 | 8 | 13 | 27 | 28 | 1 | 1 | 14 | 13 | 19 | 29 | 2 | 4 | 3 | 14 | 54 | 55 | 1 |
| 1 | 14 | 12 | 17 | 21 | 5 | -1 | 4 | 13 | 150 | 153 | 1 | 6 | 8 | 13 | 30 | 25 | 2 | 2 | 14 | 13 | 12 | 3 | 7 | 5 | 3 | 14 | 89 | 80 | 1 |
| 2 | 14 | 12 | 34 | 40 | 5 | 0 | 4 | 13 | 139 | 134 | 1 | -11 | 9 | 13 | 0 | 3 | 1 | 3 | 14 | 13 | 11 | 3 | 5 | 6 | 3 | 14 | 51 | 55 | 1 |
| -7 | 15 | 12 | 8 | 8 | 2 | 1 | 4 | 13 | 14 | 23 | 1 | -10 | 9 | 13 | 8 | 2 | 8 | -7 | 15 | 13 | 9 | 8 | 5 | -11 | 4 | 14 | 13 | 4 | 4 |
| -6 | 15 | 12 | 27 | 36 | 1 | 2 | 4 | 13 | 115 | 115 | 1 | -9 | 9 | 13 | 58 | 55 | 1 | -6 | 15 | 13 | 36 | 36 | 1 | -9 | 4 | 14 | 17 | 3 | 2 |
| -5 | 15 | 12 | 14 | 14 | 2 | 3 | 4 | 13 | 43 | 43 | 1 | -8 | 9 | 13 | 7 | 11 | 7 | -5 | 15 | 13 | 48 | 49 | 1 | -8 | 4 | 14 | 19 | 24 | 1 |
| -4 | 15 | 12 | 20 | 19 | 2 | 4 | 4 | 13 | 16 | 22 | 2 | -7 | 9 | 13 | 39 | 43 | 1 | -4 | 15 | 13 | 37 | 37 | 1 | -7 | 4 | 14 | 51 | 55 | 1 |
| -3 | 15 | 12 | 14 | 8 | 6 | 5 | 4 | 13 | 16 | 18 | 3 | -6 | 9 | 13 | 83 | 80 | 1 | -3 | 15 | 13 | 23 | 24 | 1 | -6 | 4 | 14 | 44 | 47 | 2 |
| -2 | 15 | 12 | 12 | 6 | 2 | 6 | 4 | 13 | 36 | 48 | 2 | -5 | 9 | 13 | 7 | 11 | 6 | -2 | 15 | 13 | 19 | 15 | 1 | -5 | 4 | 14 | 115 | 116 | 2 |
| -1 | 15 | 12 | 60 | 59 | 1 | 7 | 4 | 13 | 55 | 55 | 1 | -4 | 9 | 13 | 49 | 46 | 1 | -1 | 15 | 13 | 11 | 12 | 6 | -4 | 4 | 14 | 12 | 22 | 6 |
| 0 | 15 | 12 | 15 | 19 | 4 | -12 | 5 | 13 | 34 | 31 | 1 | -3 | 9 | 13 | 21 | 24 | 2 | 0 | 15 | 13 | 10 | 9 | 4 | -3 | 4 | 14 | 108 | 110 | 2 |
| 1 | 15 | 12 | 15 | 18 | 7 | -11 | 5 | 13 | 9 | 11 | 9 | -2 | 9 | 13 | 32 | 39 | 1 | 1 | 15 | 13 | 13 | 19 | 3 | -2 | 4 | 14 | 100 | 102 | 1 |
| 2 | 15 | 12 | 26 | 34 | 8 | -10 | 5 | 13 | 31 | 23 | 1 | -1 | 9 | 13 | 91 | 87 | 1 | -5 | 16 | 13 | 23 | 23 | 2 | -1 | 4 | 14 | 66 | 74 | 1 |
| 3 | 15 | 12 | 14 | 3 | 11 | -9 | 5 | 13 | 17 | 4 | 1 | 0 | 9 | 13 | 10 | 13 | 6 | -4 | 16 | 13 | 42 | 43 | 1 | 0 | 4 | 14 | 40 | 37 | 1 |
| -5 | 16 | 12 | 12 | 12 | 1 | -8 | 5 | 13 | 27 | 31 | 2 | 1 | 9 | 13 | 64 | 64 | 2 | -3 | 16 | 13 | 17 | 8 | 2 | 1 | 4 | 14 | 120 | 117 | 1 |
| -4 | 16 | 12 | 9 | 13 | 9 | -7 | 5 | 13 | 49 | 51 | 1 | 2 | 9 | 13 | 54 | 52 | 1 | -2 | 16 | 13 | 71 | 65 | 1 | 2 | 4 | 14 | 52 | 52 | 1 |
| -3 | 16 | 12 | 10 | 13 | 4 | -6 | 5 | 13 | 69 | 66 | 1 | 3 | 9 | 13 | 0 | 13 | 1 | -1 | 16 | 13 | 25 | 28 | 1 | 4 | 4 | 14 | 16 | 13 | 6 |
| -2 | 16 | 12 | 19 | 15 | 1 | -5 | 5 | 13 | 0 | 7 | 1 | 4 | 9 | 13 | 25 | 24 | 1 | 0 | 16 | 13 | 8 | 13 | 8 | 5 | 4 | 14 | 52 | 52 | 1 |
| -1 | 16 | 12 | 42 | 48 | 2 | -4 | 5 | 13 | 101 | 98 | 1 | 5 | 9 | 13 | 41 | 50 | 1 | -12 | 0 | 14 | 0 | 7 | 1 | 7 | 4 | 14 | 18 | 14 | 5 |
| 0 | 16 | 12 | 14 | 18 | 13 | -3 | 5 | 13 | 81 | 88 | 1 | 6 | 9 | 13 | 67 | 57 | 1 | -9 | 0 | 14 | 56 | 62 | 1 | -12 | 5 | 14 | 13 | 1 | 5 |
| 1 | 16 | 12 | 0 | 12 | 1 | -2 | 5 | 13 | 22 | 16 | 3 | -11 | 10 | 13 | 11 | 2 | 6 | -8 | 0 | 14 | 31 | 31 | 1 | -11 | 5 | 14 | 23 | 20 | 1 |
| -4 | 17 | 12 | 10 | 2 | 2 | -1 | 5 | 13 | 99 | 102 | 1 | -10 | 10 | 13 | 10 | 1 | 6 | -7 | 0 | 14 | 18 | 24 | 2 | -10 | 5 | 14 | 44 | 39 | 1 |
| -3 | 17 | 12 | 13 | 15 | 2 | 0 | 5 | 13 | 83 | 81 | 3 | -8 | 10 | 13 | 32 | 31 | 8 | -6 | 0 | 14 | 113 | 112 | 1 | -9 | 5 | 14 | 96 | 99 | 10 |
| -2 | 17 | 12 | 29 | 32 | 1 | 1 | 5 | 13 | 46 | 48 | 1 | -7 | 10 | 13 | 9 | 10 | 3 | -5 | 0 | 14 | 12 | 5 | 5 | -8 | 5 | 14 | 0 | 12 | 1 |
| -10 | 1 | 13 | 26 | 29 | 2 | 2 | 5 | 13 | 13 | 6 | 2 | -6 | 10 | 13 | 7 | 1 | 6 | -4 | 0 | 14 | 64 | 68 | 1 | -7 | 5 | 14 | 12 | 8 | 7 |
| -9 | 1 | 13 | 58 | 59 | 1 | 3 | 5 | 13 | 5 | 12 | 5 | -5 | 10 | 13 | 26 | 25 | 3 | -3 | 0 | 14 | 137 | 136 | 1 | -6 | 5 | 14 | 129 | 129 | 2 |
| -8 | 1 | 13 | 20 | 24 | 2 | 4 | 5 | 13 | 12 | 3 | 5 | -4 | 10 | 13 | 37 | 34 | 1 | -2 | 0 | 14 | 7 | 7 | 7 | -5 | 5 | 14 | 49 | 48 | 1 |
| -7 | 1 | 13 | 24 | 25 | 1 | 5 | 5 | 13 | 48 | 41 | 1 | -3 | 10 | 13 | 47 | 49 | 1 | -1 | 0 | 14 | 54 | 48 | 1 | -4 | 5 | 14 | 65 | 62 | 1 |
| -6 | 1 | 13 | 110 | 108 | 1 | 6 | 5 | 13 | 40 | 38 | 2 | -2 | 10 | 13 | 41 | 42 | 1 | 0 | 0 | 14 | 26 | 27 | 1 | -3 | 5 | 14 | 25 | 31 | 4 |
| -5 | 1 | 13 | 153 | 149 | 4 | 7 | 5 | 13 | 16 | 18 | 4 | -1 | 10 | 13 | 129 | 127 | 1 | 1 | 0 | 14 | 17 | 15 | 2 | -2 | 5 | 14 | 119 | 113 | 1 |
| -4 | 1 | 13 | 8 | 14 | 7 | -12 | 6 | 13 | 0 | 2 | 1 | 0 | 10 | 13 | 7 | 0 | 7 | 2 | 0 | 14 | 93 | 93 | 1 | -1 | 5 | 14 | 123 | 117 | 2 |
| -3 | 1 | 13 | 168 | 171 | 1 | -11 | 6 | 13 | 0 | 1 | 1 | 1 | 10 | 13 | 21 | 23 | 1 | 3 | 0 | 14 | 170 | 157 | 1 | 0 | 5 | 14 | 0 | 2 | 1 |
| -2 | 1 | 13 | 225 | 226 | 1 | -10 | 6 | 13 | 17 | 3 | 2 | 2 | 10 | 13 | 88 | 84 | 1 | 4 | 0 | 14 | 78 | 73 | 1 | 1 | 5 | 14 | 11 | 1 | 3 |
| -1 | 1 | 13 | 172 | 174 | 1 | -9 | 6 | 13 | 47 | 50 | 1 | 3 | 10 | 13 | 49 | 50 | 1 | 5 | 0 | 14 | 57 | 52 | 1 | 2 | 5 | 14 | 10 | 15 | 9 |
| 0 | 1 | 13 | 125 | 125 | 1 | -8 | 6 | 13 | 8 | 9 | 7 | 4 | 10 | 13 | 23 | 20 | 1 | 6 | 0 | 14 | 0 | 11 | 1 | 3 | 5 | 14 | 18 | 18 | 3 |
| 1 | 1 | 13 | 60 | 63 | 1 | -7 | 6 | 13 | 12 | 16 | 2 | 5 | 10 | 13 | 19 | 22 | 2 | -11 | 1 | 14 | 14 | 10 | 3 | 4 | 5 | 14 | 18 | 21 | 10 |
| 2 | 1 | 13 | 13 | 19 | 2 | -6 | 6 | 13 | 19 | 11 | 1 | -10 | 11 | 13 | 25 | 24 | 1 | -10 | 1 | 14 | 17 | 1 | 4 | 5 | 5 | 14 | 32 | 30 | 3 |
| 3 | 1 | 13 | 134 | 125 | 1 | -5 | 6 | 13 | 32 | 39 | 1 | -9 | 11 | 13 | 11 | 14 | 5 | -9 | 1 | 14 | 19 | 18 | 3 | 6 | 5 | 14 | 27 | 27 | 2 |
| 4 | 1 | 13 | 40 | 44 | 2 | -4 | 6 | 13 | 84 | 79 | 1 | -8 | 11 | 13 | 31 | 31 | 1 | -8 | 1 | 14 | 28 | 31 | 1 | -12 | 6 | 14 | 26 | 22 | 2 |
| 5 | 1 | 13 | 99 | 96 | 1 | -3 | 6 | 13 | 34 | 33 | 1 | -7 | 11 | 13 | 26 | 24 | 1 | -7 | 1 | 14 | 42 | 42 | 1 | -11 | 6 | 14 | 16 | 10 | 3 |
| 6 | 1 | 13 | 0 | 3 | 1 | -2 | 6 | 13 | 58 | 63 | 1 | -6 | 11 | 13 | 13 | 9 | 2 | -6 | 1 | 14 | 98 | 90 | 1 | -10 | 6 | 14 | 79 | 78 | 1 |
| -11 | 2 | 13 | 35 | 37 | 1 | -1 | 6 | 13 | 45 | 53 | 1 | -5 | 11 | 13 | 66 | 64 | 1 | -5 | 1 | 14 | 77 | 82 | 1 | -9 | 6 | 14 | 62 | 59 | 1 |
| -10 | 2 | 13 | 36 | 39 | 2 | 0 | 6 | 13 | 10 | 6 | 2 | -4 | 11 | 13 | 13 | 10 | 2 | -4 | 1 | 14 | 8 | 7 | 8 | -8 | 6 | 14 | 10 | 6 | 3 |
| -9 | 2 | 13 | 11 | 11 | 11 | 1 | 6 | 13 | 11 | 12 | 2 | -3 | 11 | 13 | 15 | 9 | 2 | -3 | 1 | 14 | 62 | 65 | 1 | -7 | 6 | 14 | 10 | 10 | 3 |
| -8 | 2 | 13 | 14 | 17 | 2 | 2 | 6 | 13 | 58 | 63 | 1 | -2 | 11 | 13 | 15 | 13 | 3 | -2 | 1 | 14 | 48 | 55 | 1 | -6 | 6 | 14 | 28 | 25 | 1 |
| -7 | 2 | 13 | 28 | 31 | 1 | 3 | 6 | 13 | 90 | 86 | 3 | -1 | 11 | 13 | 31 | 24 | 4 | -1 | 1 | 14 | 25 | 26 | 2 | -5 | 6 | 14 | 78 | 77 | 1 |
| -6 | 2 | 13 | 100 | 104 | 1 | 4 | 6 | 13 | 19 | 21 | 2 | 0 | 11 | 13 | 30 | 26 | 1 | 0 | 1 | 14 | 41 | 39 | 1 | -4 | 6 | 14 | 79 | 77 | 1 |
| -5 | 2 | 13 | 201 | 191 | 1 | 5 | 6 | 13 | 12 | 10 | 3 | 1 | 11 | 13 | 8 | 6 | 8 | 1 | 1 | 14 | 64 | 60 | 1 | -3 | 6 | 14 | 52 | 54 | 1 |
| -4 | 2 | 13 | 42 | 44 | 1 | 6 | 6 | 13 | 12 | 15 | 6 | 2 | 11 | 13 | 47 | 44 | 1 | 3 | 1 | 14 | 47 | 45 | 1 | -2 | 6 | 14 | 102 | 102 | 2 |
| -3 | 2 | 13 | 129 | 135 | 1 | 7 | 6 | 13 | 14 | 8 | 6 | 3 | 11 | 13 | 19 | 19 | 1 | 4 | 1 | 14 | 69 | 69 | 3 | -1 | 6 | 14 | 13 | 20 | 2 |
| -2 | 2 | 13 | 166 | 172 | 1 | -12 | 7 | 13 | 12 | 13 | 6 | 4 | 11 | 13 | 59 | 55 | 1 | 5 | 1 | 14 | 39 | 37 | 1 | 0 | 6 | 14 | 63 | 58 | 1 |
| -1 | 2 | 13 | 45 | 53 | 1 | -11 | 7 | 13 | 4 | 3 | 4 | 5 | 11 | 13 | 30 | 26 | 1 | 6 | 1 | 14 | 17 | 13 | 6 | 1 | 6 | 14 | 9 | 10 | 5 |
| 0 | 2 | 13 | 115 | 111 | 1 | -10 | 7 | 13 | 13 | 11 | 3 | -10 | 12 | 13 | 41 | 43 | 1 | -12 | 2 | 14 | 19 | 23 | 4 | 2 | 6 | 14 | 23 | 27 | 3 |
| 1 | 2 | 13 | 29 | 32 | 1 | -9 | 7 | 13 | 68 | 61 | 1 | -9 | 12 | 13 | 48 | 44 | 1 | -11 | 2 | 14 | 17 | 11 | 5 | 3 | 6 | 14 | 0 | 9 | 1 |
| 2 | 2 | 13 | 82 | 87 | 1 | -8 | 7 | 13 | 12 | 18 | 11 | -8 | 12 | 13 | 14 | 15 | 2 | -10 | 2 | 14 | 44 | 49 | 1 | 4 | 6 | 14 | 98 | 93 | 1 |
| 3 | 2 | 13 | 42 | 40 | 1 | -7 | 7 | 13 | 0 | 7 | 1 | -7 | 12 | 13 | 24 | 23 | 1 | -9 | 2 | 14 | 83 | 84 | 1 | 5 | 6 | 14 | 24 | 25 | 1 |
| 6 | 2 | 13 | 37 | 36 | 1 | -6 | 7 | 1 | | | | | | | | | | | | | | | | | | | | | |

Table 10.

Observed and calculated structure factors for pchm26

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|-----|----|----|------|------|-----|-----|----|----|------|------|-----|-----|---|----|------|------|-----|-----|----|----|------|------|-----|-----|---|----|------|------|-----|
| -3 | 8 | 14 | 23 | 30 | 1 | -5 | 14 | 14 | 31 | 30 | 1 | 4 | 4 | 15 | 52 | 51 | 1 | 3 | 9 | 15 | 19 | 6 | 2 | -3 | 1 | 16 | 55 | 47 | 1 |
| -2 | 8 | 14 | 68 | 67 | 3 | -4 | 14 | 14 | 58 | 54 | 1 | 5 | 4 | 15 | 60 | 61 | 4 | 4 | 9 | 15 | 20 | 21 | 4 | -2 | 1 | 16 | 41 | 42 | 1 |
| -1 | 8 | 14 | 51 | 53 | 1 | -3 | 14 | 14 | 22 | 27 | 1 | 6 | 4 | 15 | 19 | 18 | 5 | -10 | 10 | 15 | 12 | 5 | 4 | -1 | 1 | 16 | 55 | 58 | 1 |
| 0 | 8 | 14 | 10 | 12 | 3 | -2 | 14 | 14 | 15 | 13 | 2 | -12 | 5 | 15 | 48 | 44 | 1 | -9 | 10 | 15 | 12 | 3 | 11 | 0 | 1 | 16 | 47 | 52 | 1 |
| 1 | 8 | 14 | 22 | 25 | 2 | -1 | 14 | 14 | 10 | 8 | 3 | -11 | 5 | 15 | 10 | 10 | 9 | -8 | 10 | 15 | 23 | 24 | 1 | 1 | 1 | 16 | 24 | 17 | 3 |
| 2 | 8 | 14 | 13 | 6 | 2 | 0 | 14 | 14 | 10 | 4 | 4 | -10 | 5 | 15 | 49 | 50 | 1 | -7 | 10 | 15 | 19 | 22 | 1 | 2 | 1 | 16 | 57 | 59 | 1 |
| 3 | 8 | 14 | 9 | 7 | 4 | 1 | 14 | 14 | 37 | 47 | 1 | -9 | 5 | 15 | 25 | 26 | 4 | -6 | 10 | 15 | 17 | 16 | 2 | 3 | 1 | 16 | 55 | 55 | 2 |
| 4 | 8 | 14 | 58 | 50 | 1 | 2 | 14 | 14 | 30 | 37 | 2 | -8 | 5 | 15 | 12 | 12 | 12 | -5 | 10 | 15 | 16 | 17 | 2 | 4 | 1 | 16 | 19 | 10 | 3 |
| 5 | 8 | 14 | 23 | 16 | 2 | -6 | 15 | 14 | 13 | 5 | 5 | -7 | 5 | 15 | 20 | 18 | 2 | -4 | 10 | 15 | 8 | 6 | 5 | 5 | 1 | 16 | 52 | 49 | 2 |
| 6 | 8 | 14 | 0 | 3 | 1 | -5 | 15 | 14 | 13 | 5 | 2 | -6 | 5 | 15 | 131 | 126 | 1 | -3 | 10 | 15 | 12 | 5 | 11 | -12 | 2 | 16 | 2 | 7 | 2 |
| -11 | 9 | 14 | 29 | 28 | 1 | -4 | 15 | 14 | 0 | 8 | 1 | -5 | 5 | 15 | 148 | 146 | 1 | -2 | 10 | 15 | 16 | 12 | 2 | -11 | 2 | 16 | 16 | 5 | 5 |
| -10 | 9 | 14 | 13 | 10 | 4 | -3 | 15 | 14 | 15 | 22 | 2 | -4 | 5 | 15 | 45 | 48 | 1 | -1 | 10 | 15 | 35 | 36 | 2 | -10 | 2 | 16 | 21 | 21 | 2 |
| -9 | 9 | 14 | 12 | 6 | 3 | -2 | 15 | 14 | 26 | 25 | 1 | -3 | 5 | 15 | 90 | 96 | 1 | 0 | 10 | 15 | 14 | 4 | 2 | -9 | 2 | 16 | 24 | 27 | 2 |
| -8 | 9 | 14 | 12 | 11 | 4 | 0 | 15 | 14 | 12 | 17 | 12 | -2 | 5 | 15 | 66 | 65 | 1 | 1 | 10 | 15 | 0 | 0 | 1 | -8 | 2 | 16 | 35 | 32 | 1 |
| -7 | 9 | 14 | 9 | 13 | 7 | -4 | 16 | 14 | 10 | 9 | 5 | -1 | 5 | 15 | 100 | 100 | 1 | 2 | 10 | 15 | 0 | 6 | 1 | -7 | 2 | 16 | 16 | 9 | 5 |
| -6 | 9 | 14 | 35 | 35 | 1 | -3 | 16 | 14 | 24 | 9 | 3 | 0 | 5 | 15 | 29 | 34 | 1 | 3 | 10 | 15 | 11 | 1 | 6 | -6 | 2 | 16 | 37 | 35 | 1 |
| -5 | 9 | 14 | 12 | 1 | 11 | -2 | 16 | 14 | 25 | 12 | 3 | 1 | 5 | 15 | 21 | 23 | 2 | 4 | 10 | 15 | 23 | 25 | 2 | -5 | 2 | 16 | 21 | 20 | 1 |
| -4 | 9 | 14 | 30 | 30 | 1 | -11 | 1 | 15 | 44 | 40 | 2 | 2 | 5 | 15 | 82 | 81 | 1 | -9 | 11 | 15 | 16 | 8 | 8 | -4 | 2 | 16 | 12 | 13 | 2 |
| -3 | 9 | 14 | 51 | 55 | 1 | -10 | 1 | 15 | 35 | 34 | 1 | 3 | 5 | 15 | 88 | 46 | 1 | -8 | 11 | 15 | 17 | 13 | 2 | -3 | 2 | 16 | 25 | 25 | 1 |
| -2 | 9 | 14 | 54 | 55 | 1 | -9 | 1 | 15 | 17 | 18 | 2 | 4 | 5 | 15 | 53 | 51 | 1 | -7 | 11 | 15 | 26 | 27 | 1 | -2 | 2 | 16 | 14 | 18 | 1 |
| -1 | 9 | 14 | 29 | 31 | 2 | -8 | 1 | 15 | 24 | 29 | 1 | 5 | 5 | 15 | 21 | 19 | 3 | -6 | 11 | 15 | 13 | 5 | 5 | -1 | 2 | 16 | 19 | 22 | 1 |
| 0 | 9 | 14 | 11 | 7 | 3 | -7 | 1 | 15 | 10 | 1 | 3 | -6 | 5 | 15 | 73 | 71 | 1 | -5 | 11 | 15 | 14 | 16 | 2 | 0 | 2 | 16 | 27 | 28 | 2 |
| 1 | 9 | 14 | 8 | 16 | 5 | -6 | 1 | 15 | 14 | 11 | 1 | -12 | 6 | 15 | 15 | 16 | 7 | -4 | 11 | 15 | 51 | 49 | 1 | 1 | 2 | 16 | 16 | 8 | 4 |
| 2 | 9 | 14 | 56 | 56 | 1 | -5 | 1 | 15 | 12 | 13 | 2 | -11 | 6 | 15 | 0 | 2 | 1 | -3 | 11 | 15 | 42 | 44 | 2 | 2 | 2 | 16 | 13 | 1 | 9 |
| 3 | 9 | 14 | 22 | 28 | 1 | -3 | 1 | 15 | 81 | 83 | 1 | -10 | 6 | 15 | 77 | 71 | 1 | -2 | 11 | 15 | 11 | 1 | 4 | 3 | 2 | 16 | 46 | 45 | 5 |
| 4 | 9 | 14 | 15 | 7 | 3 | -2 | 1 | 15 | 17 | 11 | 1 | -9 | 6 | 15 | 51 | 50 | 1 | -1 | 11 | 15 | 52 | 54 | 1 | 4 | 2 | 16 | 22 | 19 | 1 |
| 5 | 9 | 14 | 56 | 57 | 14 | -1 | 1 | 15 | 9 | 18 | 5 | -8 | 6 | 15 | 7 | 3 | 7 | 0 | 11 | 15 | 18 | 17 | 2 | 5 | 2 | 16 | 25 | 23 | 2 |
| -10 | 10 | 14 | 14 | 6 | 4 | 0 | 1 | 15 | 13 | 12 | 2 | -7 | 6 | 15 | 21 | 16 | 2 | 1 | 11 | 15 | 12 | 4 | 4 | -12 | 3 | 16 | 28 | 28 | 2 |
| -9 | 10 | 14 | 39 | 32 | 1 | 1 | 1 | 15 | 129 | 129 | 1 | -6 | 6 | 15 | 30 | 21 | 2 | 2 | 11 | 15 | 26 | 28 | 4 | -11 | 3 | 16 | 28 | 27 | 3 |
| -8 | 10 | 14 | 26 | 31 | 1 | 2 | 1 | 15 | 32 | 34 | 4 | -5 | 6 | 15 | 103 | 101 | 3 | 3 | 11 | 15 | 13 | 21 | 4 | -10 | 3 | 16 | 31 | 30 | 1 |
| -7 | 10 | 14 | 12 | 14 | 3 | 3 | 1 | 15 | 39 | 41 | 2 | -4 | 6 | 15 | 31 | 37 | 2 | -9 | 12 | 15 | 20 | 22 | 2 | -9 | 3 | 16 | 100 | 93 | 1 |
| -6 | 10 | 14 | 8 | 9 | 7 | 4 | 1 | 15 | 0 | 7 | 1 | -3 | 6 | 15 | 88 | 92 | 4 | -8 | 12 | 15 | 20 | 18 | 1 | -8 | 3 | 16 | 13 | 17 | 6 |
| -5 | 10 | 14 | 12 | 12 | 2 | 5 | 1 | 15 | 18 | 20 | 2 | -2 | 6 | 15 | 84 | 80 | 2 | -7 | 12 | 15 | 19 | 18 | 2 | -7 | 3 | 16 | 40 | 32 | 1 |
| -4 | 10 | 14 | 9 | 10 | 5 | 6 | 1 | 15 | 30 | 34 | 3 | -1 | 6 | 15 | 6 | 2 | 6 | -6 | 12 | 15 | 8 | 1 | 8 | -6 | 3 | 16 | 43 | 40 | 1 |
| -3 | 10 | 14 | 19 | 19 | 1 | -12 | 2 | 15 | 0 | 7 | 1 | 0 | 6 | 15 | 66 | 68 | 2 | -5 | 12 | 15 | 8 | 15 | 8 | -5 | 3 | 16 | 53 | 57 | 1 |
| -2 | 10 | 14 | 60 | 57 | 2 | -11 | 2 | 15 | 14 | 5 | 8 | 1 | 6 | 15 | 44 | 40 | 1 | -4 | 12 | 15 | 18 | 17 | 1 | -4 | 3 | 16 | 36 | 34 | 1 |
| -1 | 10 | 14 | 31 | 35 | 1 | -10 | 2 | 15 | 111 | 103 | 1 | 2 | 6 | 15 | 58 | 61 | 1 | -3 | 12 | 15 | 18 | 13 | 2 | -3 | 3 | 16 | 14 | 21 | 1 |
| 0 | 10 | 14 | 25 | 22 | 3 | -9 | 2 | 15 | 18 | 19 | 2 | 3 | 6 | 15 | 23 | 20 | 1 | -2 | 12 | 15 | 21 | 14 | 1 | -2 | 3 | 16 | 13 | 16 | 2 |
| 1 | 10 | 14 | 45 | 40 | 1 | -8 | 2 | 15 | 11 | 15 | 3 | 4 | 6 | 15 | 29 | 31 | 1 | -1 | 12 | 15 | 12 | 18 | 6 | -1 | 3 | 16 | 12 | 14 | 2 |
| 2 | 10 | 14 | 48 | 42 | 1 | -7 | 2 | 15 | 9 | 3 | 5 | 5 | 6 | 15 | 14 | 7 | 10 | 0 | 12 | 15 | 0 | 4 | 1 | 0 | 3 | 16 | 15 | 14 | 2 |
| 3 | 10 | 14 | 19 | 16 | 2 | -6 | 2 | 15 | 136 | 136 | 1 | 6 | 6 | 15 | 14 | 10 | 7 | 1 | 12 | 15 | 39 | 36 | 1 | 1 | 3 | 16 | 44 | 41 | 1 |
| 4 | 10 | 14 | 18 | 8 | 2 | -5 | 2 | 15 | 77 | 70 | 3 | -11 | 7 | 15 | 12 | 9 | 10 | 2 | 12 | 15 | 12 | 8 | 8 | 2 | 3 | 16 | 123 | 120 | 5 |
| 5 | 10 | 14 | 32 | 33 | 2 | -4 | 2 | 15 | 57 | 64 | 3 | -10 | 7 | 15 | 75 | 75 | 1 | 3 | 12 | 15 | 54 | 44 | 1 | 3 | 3 | 16 | 13 | 7 | 4 |
| -10 | 11 | 14 | 17 | 17 | 3 | -3 | 2 | 15 | 68 | 64 | 1 | -9 | 7 | 15 | 71 | 65 | 1 | -8 | 13 | 15 | 14 | 8 | 4 | 4 | 3 | 16 | 73 | 69 | 2 |
| -9 | 11 | 14 | 14 | 19 | 4 | -2 | 2 | 15 | 8 | 12 | 6 | -8 | 7 | 15 | 19 | 21 | 2 | -7 | 13 | 15 | 39 | 38 | 1 | 5 | 3 | 16 | 36 | 40 | 3 |
| -8 | 11 | 14 | 8 | 4 | 8 | -1 | 2 | 15 | 64 | 70 | 1 | -7 | 7 | 15 | 18 | 19 | 5 | -6 | 13 | 15 | 24 | 29 | 1 | -12 | 4 | 16 | 12 | 6 | 11 |
| -7 | 11 | 14 | 40 | 33 | 1 | 0 | 2 | 15 | 10 | 10 | 3 | -6 | 7 | 15 | 54 | 51 | 1 | -5 | 13 | 15 | 36 | 32 | 1 | -11 | 4 | 16 | 20 | 22 | 2 |
| -6 | 11 | 14 | 75 | 70 | 3 | 1 | 2 | 15 | 107 | 100 | 1 | -5 | 7 | 15 | 119 | 117 | 3 | -4 | 13 | 15 | 13 | 9 | 6 | -10 | 4 | 16 | 49 | 41 | 1 |
| -5 | 11 | 14 | 9 | 13 | 9 | 2 | 2 | 15 | 28 | 28 | 3 | -4 | 7 | 15 | 53 | 55 | 1 | -3 | 13 | 15 | 13 | 4 | 3 | -9 | 4 | 16 | 23 | 20 | 2 |
| -4 | 11 | 14 | 10 | 8 | 3 | 3 | 2 | 15 | 7 | 2 | 7 | -3 | 7 | 15 | 76 | 78 | 1 | -1 | 13 | 15 | 29 | 36 | 1 | -8 | 4 | 16 | 63 | 57 | 1 |
| -3 | 11 | 14 | 67 | 65 | 3 | 4 | 2 | 15 | 35 | 33 | 1 | -2 | 7 | 15 | 152 | 154 | 1 | 0 | 13 | 15 | 30 | 37 | 2 | -7 | 4 | 16 | 66 | 64 | 1 |
| -2 | 11 | 14 | 17 | 10 | 2 | 5 | 2 | 15 | 0 | 8 | 1 | -1 | 7 | 15 | 101 | 92 | 1 | 1 | 13 | 15 | 16 | 17 | 3 | -6 | 4 | 16 | 40 | 36 | 1 |
| -1 | 11 | 14 | 78 | 71 | 1 | 6 | 2 | 15 | 37 | 35 | 2 | 0 | 7 | 15 | 25 | 25 | 1 | -7 | 14 | 15 | 13 | 7 | 3 | -5 | 4 | 16 | 42 | 47 | 1 |
| 0 | 11 | 14 | 25 | 26 | 1 | -12 | 3 | 15 | 17 | 8 | 3 | 1 | 7 | 15 | 38 | 35 | 1 | -6 | 14 | 15 | 15 | 10 | 3 | -4 | 4 | 16 | 27 | 37 | 1 |
| 1 | 11 | 14 | 97 | 89 | 1 | -11 | 3 | 15 | 19 | 15 | 2 | 2 | 7 | 15 | 61 | 66 | 1 | -5 | 14 | 15 | 11 | 2 | 4 | -3 | 4 | 16 | 30 | 32 | 1 |
| 2 | 11 | 14 | 0 | 0 | 1 | -10 | 3 | 15 | 15 | 0 | 2 | 3 | 7 | 15 | 64 | 60 | 2 | -4 | 14 | 15 | 8 | 9 | 7 | -2 | 4 | 16 | 12 | 17 | 2 |
| 3 | 11 | 14 | 58 | 55 | 1 | -9 | 3 | 15 | 14 | 8 | 2 | 4 | 7 | 15 | 16 | 18 | 3 | -3 | 14 | 15 | 13 | 6 | 7 | -1 | 4 | 16 | 12 | 12 | 3 |
| 4 | 11 | 14 | 0 | 6 | 1 | -8 | 3 | 15 | 33 | 34 | 1 | -11 | 8 | 15 | 0 | 6 | 1 | -2 | 14 | 15 | 55 | 42 | 1 | 0 | 4 | 16 | 67 | 69 | 1 |
| -9 | 12 | 14 | 9 | 11 | 6 | -7 | 3 | 15 | 22 | 23 | 1 | -10 | 8 | 15 | 44 | 45 | 4 | -1 | 14 | 15 | 8 | 7 | 7 | 1 | 4 | 16 | 13 | 6 | 2 |
| -8 | 12 | 14 | 9 | 2 | 5 | -6 | 3 | 15 | 53 | 48 | | | | | | | | | | | | | | | | | | | |

Table 10.

Observed and calculated structure factors for pchm26

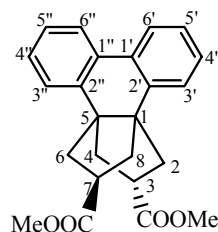
| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|-----|----|----|------|------|-----|-----|----|----|------|------|-----|-----|---|----|------|------|-----|-----|----|----|------|------|-----|-----|---|----|------|------|-----|
| -5 | 6 | 16 | 10 | 7 | 3 | -1 | 12 | 16 | 19 | 23 | 5 | -8 | 5 | 17 | 16 | 17 | 4 | -5 | 11 | 17 | 9 | 1 | 9 | -8 | 4 | 18 | 28 | 34 | 1 |
| -4 | 6 | 16 | 37 | 39 | 1 | 0 | 12 | 16 | 15 | 14 | 3 | -7 | 5 | 17 | 44 | 43 | 2 | -4 | 11 | 17 | 12 | 13 | 3 | -7 | 4 | 18 | 28 | 32 | 1 |
| -3 | 6 | 16 | 55 | 54 | 3 | 1 | 12 | 16 | 60 | 56 | 1 | -6 | 5 | 17 | 8 | 8 | 7 | -3 | 11 | 17 | 19 | 25 | 2 | -6 | 4 | 18 | 18 | 13 | 2 |
| -2 | 6 | 16 | 123 | 124 | 1 | 2 | 12 | 16 | 45 | 32 | 2 | -5 | 5 | 17 | 37 | 43 | 1 | -2 | 11 | 17 | 21 | 22 | 2 | -5 | 4 | 18 | 12 | 9 | 3 |
| -1 | 6 | 16 | 0 | 7 | 1 | -7 | 13 | 16 | 11 | 3 | 4 | -4 | 5 | 17 | 34 | 32 | 1 | -1 | 11 | 17 | 10 | 16 | 5 | -4 | 4 | 18 | 37 | 38 | 1 |
| 0 | 6 | 16 | 47 | 44 | 1 | -6 | 13 | 16 | 17 | 11 | 2 | -3 | 5 | 17 | 15 | 14 | 2 | 0 | 11 | 17 | 12 | 15 | 6 | -3 | 4 | 18 | 36 | 38 | 1 |
| 1 | 6 | 16 | 15 | 4 | 2 | -5 | 13 | 16 | 13 | 0 | 3 | -2 | 5 | 17 | 35 | 34 | 1 | 1 | 11 | 17 | 17 | 0 | 3 | -2 | 4 | 18 | 0 | 3 | 1 |
| 2 | 6 | 16 | 53 | 53 | 2 | -4 | 13 | 16 | 15 | 14 | 2 | -1 | 5 | 17 | 6 | 4 | 6 | -7 | 12 | 17 | 31 | 34 | 3 | -1 | 4 | 18 | 12 | 21 | 9 |
| 3 | 6 | 16 | 24 | 23 | 5 | -3 | 13 | 16 | 19 | 15 | 2 | 0 | 5 | 17 | 18 | 21 | 2 | -6 | 12 | 17 | 18 | 21 | 2 | 0 | 4 | 18 | 6 | 0 | 5 |
| 4 | 6 | 16 | 15 | 14 | 4 | -2 | 13 | 16 | 14 | 14 | 3 | 1 | 5 | 17 | 18 | 7 | 3 | -5 | 12 | 17 | 16 | 13 | 3 | 1 | 4 | 18 | 22 | 16 | 3 |
| -11 | 7 | 16 | 0 | 9 | 1 | -1 | 13 | 16 | 24 | 26 | 1 | 2 | 5 | 17 | 31 | 29 | 3 | -4 | 12 | 17 | 14 | 7 | 3 | 2 | 4 | 18 | 25 | 29 | 3 |
| -10 | 7 | 16 | 18 | 1 | 7 | 0 | 13 | 16 | 16 | 20 | 6 | 3 | 5 | 17 | 25 | 26 | 1 | -3 | 12 | 17 | 21 | 11 | 5 | 3 | 4 | 18 | 13 | 2 | 8 |
| -9 | 7 | 16 | 18 | 21 | 3 | -5 | 14 | 16 | 31 | 30 | 1 | 4 | 5 | 17 | 65 | 70 | 7 | -2 | 12 | 17 | 33 | 33 | 3 | -11 | 5 | 18 | 26 | 29 | 4 |
| -8 | 7 | 16 | 30 | 32 | 5 | -4 | 14 | 16 | 7 | 9 | 7 | -11 | 6 | 17 | 25 | 14 | 3 | -1 | 12 | 17 | 26 | 26 | 1 | -10 | 5 | 18 | 32 | 30 | 2 |
| -7 | 7 | 16 | 73 | 72 | 1 | -3 | 14 | 16 | 31 | 33 | 2 | -10 | 6 | 17 | 54 | 51 | 1 | 0 | 12 | 17 | 19 | 23 | 4 | -9 | 5 | 18 | 50 | 51 | 1 |
| -6 | 7 | 16 | 18 | 8 | 1 | -2 | 14 | 16 | 17 | 5 | 4 | -9 | 6 | 17 | 39 | 40 | 1 | -6 | 13 | 17 | 26 | 28 | 2 | -8 | 5 | 18 | 12 | 27 | 7 |
| -5 | 7 | 16 | 106 | 104 | 1 | -11 | 1 | 17 | 34 | 36 | 1 | -8 | 6 | 17 | 11 | 3 | 4 | -5 | 13 | 17 | 9 | 13 | 9 | -7 | 5 | 18 | 16 | 8 | 2 |
| -4 | 7 | 16 | 62 | 61 | 1 | -10 | 1 | 17 | 59 | 59 | 1 | -7 | 6 | 17 | 25 | 26 | 1 | -4 | 13 | 17 | 16 | 4 | 3 | -6 | 5 | 18 | 75 | 72 | 1 |
| -3 | 7 | 16 | 13 | 6 | 4 | -9 | 1 | 17 | 9 | 8 | 8 | -6 | 6 | 17 | 53 | 46 | 1 | -3 | 13 | 17 | 25 | 26 | 1 | -5 | 5 | 18 | 100 | 98 | 1 |
| -2 | 7 | 16 | 30 | 28 | 3 | -8 | 1 | 17 | 25 | 25 | 1 | -5 | 6 | 17 | 8 | 1 | 5 | -2 | 13 | 17 | 9 | 15 | 8 | -4 | 5 | 18 | 60 | 61 | 1 |
| -1 | 7 | 16 | 9 | 11 | 6 | -7 | 1 | 17 | 14 | 13 | 2 | -4 | 6 | 17 | 75 | 68 | 1 | -1 | 13 | 17 | 0 | 8 | 1 | -3 | 5 | 18 | 18 | 18 | 1 |
| 0 | 7 | 16 | 32 | 35 | 1 | -6 | 1 | 17 | 44 | 45 | 1 | -3 | 6 | 17 | 35 | 33 | 1 | -11 | 0 | 18 | 0 | 11 | 1 | -2 | 5 | 18 | 29 | 30 | 2 |
| 1 | 7 | 16 | 14 | 9 | 2 | -5 | 1 | 17 | 9 | 11 | 8 | -2 | 6 | 17 | 74 | 78 | 1 | -10 | 0 | 18 | 37 | 38 | 2 | -1 | 5 | 18 | 40 | 42 | 1 |
| 2 | 7 | 16 | 28 | 28 | 1 | -4 | 1 | 17 | 13 | 6 | 2 | -1 | 6 | 17 | 17 | 28 | 11 | -9 | 0 | 18 | 29 | 32 | 2 | 0 | 5 | 18 | 20 | 17 | 2 |
| 3 | 7 | 16 | 10 | 5 | 10 | -3 | 1 | 17 | 88 | 88 | 1 | 0 | 6 | 17 | 11 | 3 | 4 | -8 | 0 | 18 | 0 | 16 | 1 | 1 | 5 | 18 | 20 | 24 | 2 |
| 4 | 7 | 16 | 9 | 3 | 9 | -2 | 1 | 17 | 131 | 126 | 1 | 1 | 6 | 17 | 51 | 46 | 1 | -7 | 0 | 18 | 33 | 37 | 1 | 2 | 5 | 18 | 87 | 86 | 6 |
| -11 | 8 | 16 | 0 | 18 | 1 | -1 | 1 | 17 | 12 | 20 | 6 | 2 | 6 | 17 | 75 | 71 | 1 | -6 | 0 | 18 | 14 | 17 | 1 | 3 | 5 | 18 | 13 | 9 | 7 |
| -10 | 8 | 16 | 40 | 32 | 1 | 0 | 1 | 17 | 8 | 12 | 8 | 3 | 6 | 17 | 45 | 43 | 1 | -5 | 0 | 18 | 14 | 17 | 5 | -10 | 6 | 18 | 18 | 16 | 8 |
| -9 | 8 | 16 | 77 | 71 | 2 | 1 | 1 | 17 | 9 | 2 | 8 | 4 | 6 | 17 | 21 | 6 | 4 | -4 | 0 | 18 | 61 | 50 | 1 | -9 | 6 | 18 | 64 | 62 | 1 |
| -8 | 8 | 16 | 28 | 28 | 1 | 2 | 1 | 17 | 0 | 5 | 1 | -10 | 7 | 17 | 35 | 34 | 1 | -3 | 0 | 18 | 89 | 82 | 1 | -8 | 6 | 18 | 22 | 20 | 3 |
| -7 | 8 | 16 | 17 | 16 | 2 | 3 | 1 | 17 | 5 | 5 | 4 | -9 | 7 | 17 | 12 | 13 | 6 | -2 | 0 | 18 | 33 | 31 | 1 | -7 | 6 | 18 | 21 | 19 | 1 |
| -6 | 8 | 16 | 51 | 50 | 1 | 4 | 1 | 17 | 32 | 32 | 3 | -8 | 7 | 17 | 23 | 24 | 2 | -1 | 0 | 18 | 0 | 9 | 1 | -6 | 6 | 18 | 21 | 19 | 1 |
| -5 | 8 | 16 | 24 | 26 | 1 | 5 | 1 | 17 | 25 | 26 | 4 | -7 | 7 | 17 | 57 | 52 | 1 | 0 | 0 | 18 | 47 | 44 | 1 | -5 | 6 | 18 | 45 | 49 | 1 |
| -4 | 8 | 16 | 34 | 37 | 2 | -12 | 2 | 17 | 23 | 30 | 3 | -6 | 7 | 17 | 15 | 12 | 2 | 1 | 0 | 18 | 173 | 163 | 1 | -4 | 6 | 18 | 34 | 40 | 1 |
| -3 | 8 | 16 | 15 | 12 | 8 | -11 | 2 | 17 | 0 | 15 | 1 | -5 | 7 | 17 | 44 | 41 | 1 | 2 | 0 | 18 | 20 | 31 | 3 | -3 | 6 | 18 | 12 | 23 | 9 |
| -2 | 8 | 16 | 81 | 86 | 1 | -10 | 2 | 17 | 61 | 58 | 1 | -4 | 7 | 17 | 72 | 69 | 1 | 3 | 0 | 18 | 19 | 16 | 3 | -2 | 6 | 18 | 67 | 70 | 3 |
| -1 | 8 | 16 | 12 | 16 | 6 | -9 | 2 | 17 | 17 | 10 | 4 | -3 | 7 | 17 | 8 | 6 | 7 | 4 | 0 | 18 | 0 | 9 | 1 | -1 | 6 | 18 | 39 | 43 | 2 |
| 0 | 8 | 16 | 22 | 16 | 2 | -8 | 2 | 17 | 39 | 36 | 2 | -2 | 7 | 17 | 32 | 33 | 2 | -11 | 1 | 18 | 25 | 34 | 2 | 0 | 6 | 18 | 45 | 47 | 1 |
| 1 | 8 | 16 | 39 | 34 | 1 | -7 | 2 | 17 | 37 | 37 | 1 | -1 | 7 | 17 | 15 | 18 | 3 | -10 | 1 | 18 | 40 | 42 | 1 | 1 | 6 | 18 | 13 | 9 | 4 |
| 2 | 8 | 16 | 31 | 26 | 3 | -6 | 2 | 17 | 19 | 15 | 1 | 0 | 7 | 17 | 20 | 22 | 4 | -9 | 1 | 18 | 8 | 7 | 7 | 3 | 6 | 18 | 39 | 36 | 2 |
| 3 | 8 | 16 | 82 | 77 | 1 | -5 | 2 | 17 | 17 | 17 | 1 | 1 | 7 | 17 | 27 | 28 | 1 | -8 | 1 | 18 | 7 | 7 | 7 | -10 | 7 | 18 | 40 | 37 | 4 |
| 4 | 8 | 16 | 0 | 1 | 1 | -4 | 2 | 17 | 33 | 36 | 4 | 2 | 7 | 17 | 74 | 63 | 2 | -7 | 1 | 18 | 24 | 23 | 3 | -9 | 7 | 18 | 17 | 18 | 8 |
| -10 | 9 | 16 | 13 | 6 | 4 | -3 | 2 | 17 | 59 | 63 | 1 | 3 | 7 | 17 | 19 | 18 | 4 | -6 | 1 | 18 | 47 | 45 | 2 | -8 | 7 | 18 | 20 | 21 | 2 |
| -9 | 9 | 16 | 32 | 29 | 1 | -2 | 2 | 17 | 44 | 45 | 1 | 4 | 7 | 17 | 29 | 29 | 2 | -5 | 1 | 18 | 33 | 29 | 4 | -7 | 7 | 18 | 45 | 44 | 1 |
| -8 | 9 | 16 | 0 | 0 | 1 | -1 | 2 | 17 | 0 | 1 | 1 | -10 | 8 | 17 | 79 | 71 | 1 | -4 | 1 | 18 | 49 | 47 | 1 | -6 | 7 | 18 | 82 | 78 | 1 |
| -7 | 9 | 16 | 32 | 31 | 2 | 0 | 2 | 17 | 25 | 32 | 1 | -9 | 8 | 17 | 7 | 0 | 7 | -3 | 1 | 18 | 18 | 13 | 2 | -5 | 7 | 18 | 19 | 17 | 1 |
| -6 | 9 | 16 | 15 | 11 | 2 | 1 | 2 | 17 | 64 | 61 | 2 | -8 | 8 | 17 | 11 | 12 | 7 | -2 | 1 | 18 | 45 | 45 | 1 | -4 | 7 | 18 | 14 | 0 | 3 |
| -5 | 9 | 16 | 25 | 26 | 1 | 2 | 2 | 17 | 60 | 58 | 1 | -7 | 8 | 17 | 39 | 39 | 1 | -1 | 1 | 18 | 71 | 63 | 1 | -3 | 7 | 18 | 7 | 7 | 6 |
| -4 | 9 | 16 | 12 | 0 | 2 | 3 | 2 | 17 | 7 | 14 | 6 | -6 | 8 | 17 | 22 | 26 | 2 | 0 | 1 | 18 | 52 | 51 | 2 | -2 | 7 | 18 | 11 | 11 | 3 |
| -3 | 9 | 16 | 12 | 4 | 3 | 4 | 2 | 17 | 41 | 41 | 1 | -5 | 8 | 17 | 14 | 12 | 6 | 1 | 1 | 18 | 14 | 11 | 3 | -1 | 7 | 18 | 14 | 14 | 2 |
| -2 | 9 | 16 | 20 | 25 | 1 | 5 | 2 | 17 | 24 | 30 | 3 | -4 | 8 | 17 | 60 | 57 | 1 | 2 | 1 | 18 | 0 | 19 | 1 | 0 | 7 | 18 | 0 | 0 | 1 |
| -1 | 9 | 16 | 38 | 37 | 1 | -11 | 3 | 17 | 0 | 9 | 1 | -3 | 8 | 17 | 134 | 130 | 3 | 3 | 1 | 18 | 0 | 5 | 1 | 1 | 7 | 18 | 31 | 30 | 2 |
| 0 | 9 | 16 | 15 | 12 | 5 | -10 | 3 | 17 | 20 | 14 | 2 | -2 | 8 | 17 | 33 | 36 | 8 | 4 | 1 | 18 | 37 | 36 | 2 | 2 | 7 | 18 | 0 | 1 | 1 |
| 1 | 9 | 16 | 15 | 8 | 2 | -9 | 3 | 17 | 18 | 16 | 2 | -1 | 8 | 17 | 26 | 24 | 1 | -11 | 2 | 18 | 24 | 25 | 5 | -9 | 8 | 18 | 53 | 52 | 5 |
| 2 | 9 | 16 | 14 | 4 | 3 | -8 | 3 | 17 | 10 | 11 | 9 | 0 | 8 | 17 | 13 | 14 | 4 | -10 | 2 | 18 | 15 | 5 | 3 | -8 | 8 | 18 | 57 | 55 | 2 |
| 3 | 9 | 16 | 46 | 44 | 2 | -7 | 3 | 17 | 53 | 57 | 1 | 1 | 8 | 17 | 25 | 28 | 1 | -9 | 2 | 18 | 60 | 58 | 1 | -7 | 8 | 18 | 22 | 22 | 1 |
| 4 | 9 | 16 | 59 | 55 | 1 | -6 | 3 | 17 | 84 | 85 | 1 | 2 | 8 | 17 | 23 | 12 | 8 | -8 | 2 | 18 | 46 | 47 | 3 | -6 | 8 | 18 | 16 | 18 | 2 |
| -10 | 10 | 16 | 13 | 10 | 12 | -5 | 3 | 17 | 42 | 43 | 1 | 3 | 8 | 17 | 69 | 68 | 1 | -7 | 2 | 18 | 57 | 56 | 1 | -5 | 8 | 18 | 43 | 46 | 1 |
| -9 | 10 | 16 | 27 | 29 | 2 | -4 | 3 | 17 | 31 | 32 | 1 | -10 | 9 | 17 | 0 | 4 | 1 | -6 | 2 | 18 | 69 | 67 | 1 | -4 | 8 | 18 | 48 | 47 | 1 |
| -8 | 10 | 16 | 12 | 11 | 3 | -3 | 3 | 17 | 19 | 18 | 1 | -9 | 9 | 17 | 22 | 21 | 2 | -5 | 2 | 18 | 18 | 18 | 1 | -3 | | | | | |

Table 10. Observed and calculated structure factors for pchm26

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|-----|----|----|------|------|-----|-----|----|----|------|------|-----|-----|----|----|------|------|-----|----|----|----|------|------|-----|----|---|----|------|------|-----|
| -6 | 11 | 18 | 14 | 5 | 3 | 2 | 4 | 19 | 38 | 36 | 6 | -3 | 11 | 19 | 15 | 9 | 3 | -4 | 5 | 20 | 86 | 82 | 1 | -7 | 4 | 21 | 9 | 3 | 8 |
| -5 | 11 | 18 | 17 | 20 | 3 | -10 | 5 | 19 | 53 | 49 | 1 | -2 | 11 | 19 | 31 | 18 | 3 | -3 | 5 | 20 | 90 | 84 | 1 | -6 | 4 | 21 | 25 | 31 | 3 |
| -4 | 11 | 18 | 15 | 3 | 2 | -9 | 5 | 19 | 53 | 52 | 1 | -10 | 0 | 20 | 45 | 51 | 1 | -2 | 5 | 20 | 32 | 31 | 7 | -5 | 4 | 21 | 33 | 35 | 2 |
| -3 | 11 | 18 | 71 | 75 | 1 | -8 | 5 | 19 | 25 | 29 | 2 | -9 | 0 | 20 | 64 | 57 | 1 | -1 | 5 | 20 | 37 | 40 | 2 | -3 | 4 | 21 | 17 | 3 | 3 |
| -2 | 11 | 18 | 18 | 20 | 2 | -7 | 5 | 19 | 37 | 37 | 1 | -8 | 0 | 20 | 33 | 27 | 1 | 0 | 5 | 20 | 18 | 18 | 5 | -2 | 4 | 21 | 12 | 19 | 7 |
| -1 | 11 | 18 | 21 | 18 | 2 | -6 | 5 | 19 | 41 | 39 | 1 | -7 | 0 | 20 | 22 | 20 | 2 | 1 | 5 | 20 | 0 | 7 | 1 | -1 | 4 | 21 | 29 | 15 | 3 |
| 0 | 11 | 18 | 12 | 1 | 11 | -5 | 5 | 19 | 53 | 53 | 3 | -6 | 0 | 20 | 24 | 23 | 2 | -9 | 6 | 20 | 24 | 29 | 3 | 0 | 4 | 21 | 36 | 40 | 3 |
| -6 | 12 | 18 | 0 | 4 | 1 | -4 | 5 | 19 | 26 | 27 | 1 | -5 | 0 | 20 | 85 | 78 | 1 | -8 | 6 | 20 | 27 | 27 | 1 | -8 | 5 | 21 | 24 | 29 | 2 |
| -5 | 12 | 18 | 30 | 29 | 7 | -3 | 5 | 19 | 45 | 46 | 5 | -4 | 0 | 20 | 15 | 18 | 3 | -7 | 6 | 20 | 20 | 11 | 4 | -7 | 5 | 21 | 75 | 71 | 1 |
| -4 | 12 | 18 | 12 | 2 | 11 | -2 | 5 | 19 | 63 | 68 | 1 | -3 | 0 | 20 | 26 | 27 | 2 | -6 | 6 | 20 | 36 | 35 | 1 | -6 | 5 | 21 | 19 | 10 | 3 |
| -3 | 12 | 18 | 20 | 28 | 2 | -1 | 5 | 19 | 15 | 16 | 4 | -2 | 0 | 20 | 20 | 27 | 4 | -5 | 6 | 20 | 57 | 53 | 1 | -5 | 5 | 21 | 14 | 5 | 3 |
| -2 | 12 | 18 | 14 | 6 | 4 | 0 | 5 | 19 | 21 | 28 | 2 | -1 | 0 | 20 | 24 | 25 | 2 | -4 | 6 | 20 | 20 | 15 | 3 | -4 | 5 | 21 | 19 | 14 | 2 |
| -1 | 1 | 19 | 15 | 23 | 4 | 1 | 5 | 19 | 12 | 4 | 8 | 0 | 0 | 20 | 49 | 51 | 1 | -3 | 6 | 20 | 119 | 114 | 9 | -3 | 5 | 21 | 35 | 37 | 1 |
| -10 | 1 | 19 | 16 | 13 | 3 | 2 | 5 | 19 | 25 | 25 | 4 | 1 | 0 | 20 | 84 | 78 | 1 | -2 | 6 | 20 | 41 | 44 | 1 | -2 | 5 | 21 | 56 | 52 | 2 |
| -9 | 1 | 19 | 8 | 5 | 8 | -10 | 6 | 19 | 16 | 14 | 5 | 2 | 0 | 20 | 31 | 30 | 2 | -1 | 6 | 20 | 33 | 40 | 1 | -1 | 5 | 21 | 15 | 23 | 7 |
| -8 | 1 | 19 | 27 | 28 | 1 | -9 | 6 | 19 | 13 | 10 | 12 | -10 | 1 | 20 | 15 | 12 | 4 | 0 | 6 | 20 | 13 | 17 | 13 | -7 | 6 | 21 | 19 | 11 | 3 |
| -7 | 1 | 19 | 21 | 19 | 3 | -8 | 6 | 19 | 31 | 29 | 1 | -9 | 1 | 20 | 20 | 20 | 3 | -8 | 7 | 20 | 32 | 35 | 4 | -6 | 7 | 21 | 16 | 16 | 15 |
| -6 | 1 | 19 | 61 | 60 | 1 | -7 | 6 | 19 | 17 | 13 | 2 | -8 | 1 | 20 | 34 | 30 | 1 | -7 | 7 | 20 | 14 | 4 | 3 | -5 | 6 | 21 | 53 | 49 | 2 |
| -5 | 1 | 19 | 15 | 11 | 11 | -6 | 6 | 19 | 112 | 106 | 1 | -7 | 1 | 20 | 37 | 35 | 1 | -6 | 7 | 20 | 38 | 41 | 1 | -4 | 6 | 21 | 67 | 67 | 1 |
| -4 | 1 | 19 | 47 | 44 | 4 | -5 | 6 | 19 | 53 | 56 | 1 | -6 | 1 | 20 | 23 | 22 | 1 | -5 | 7 | 20 | 39 | 42 | 1 | -3 | 6 | 21 | 15 | 5 | 3 |
| -3 | 1 | 19 | 12 | 19 | 3 | -4 | 6 | 19 | 9 | 5 | 9 | -5 | 1 | 20 | 16 | 3 | 6 | -4 | 7 | 20 | 36 | 31 | 2 | -2 | 6 | 21 | 29 | 29 | 2 |
| -2 | 1 | 19 | 13 | 5 | 7 | -3 | 6 | 19 | 23 | 21 | 2 | -4 | 1 | 20 | 80 | 74 | 1 | -3 | 7 | 20 | 23 | 21 | 2 | -1 | 6 | 21 | 18 | 25 | 7 |
| -1 | 1 | 19 | 35 | 37 | 1 | -2 | 6 | 19 | 44 | 43 | 5 | -3 | 1 | 20 | 38 | 42 | 1 | -2 | 7 | 20 | 13 | 0 | 4 | -7 | 7 | 21 | 0 | 11 | 1 |
| 0 | 1 | 19 | 20 | 17 | 3 | -1 | 6 | 19 | 13 | 16 | 4 | -2 | 1 | 20 | 14 | 9 | 3 | -1 | 7 | 20 | 12 | 9 | 7 | -6 | 7 | 21 | 22 | 15 | 2 |
| 1 | 1 | 19 | 65 | 64 | 1 | 0 | 6 | 19 | 11 | 8 | 7 | -1 | 1 | 20 | 16 | 27 | 3 | 0 | 7 | 20 | 24 | 29 | 5 | -5 | 7 | 21 | 20 | 8 | 2 |
| 2 | 1 | 19 | 37 | 44 | 3 | 1 | 6 | 19 | 78 | 73 | 3 | 0 | 1 | 20 | 75 | 70 | 1 | -7 | 8 | 20 | 36 | 37 | 4 | -4 | 7 | 21 | 62 | 58 | 1 |
| 3 | 1 | 19 | 18 | 21 | 4 | 2 | 6 | 19 | 13 | 5 | 4 | 1 | 1 | 20 | 52 | 46 | 2 | -6 | 8 | 20 | 14 | 3 | 3 | -3 | 7 | 21 | 0 | 3 | 1 |
| -11 | 2 | 19 | 0 | 14 | 1 | -9 | 7 | 19 | 41 | 36 | 1 | 2 | 1 | 20 | 22 | 14 | 6 | -5 | 8 | 20 | 30 | 29 | 1 | -5 | 8 | 21 | 32 | 31 | 3 |
| -10 | 2 | 19 | 37 | 36 | 1 | -8 | 7 | 19 | 17 | 20 | 3 | -10 | 2 | 20 | 13 | 8 | 5 | -4 | 8 | 20 | 50 | 50 | 3 | -4 | 8 | 21 | 15 | 26 | 6 |
| -9 | 2 | 19 | 21 | 23 | 2 | -7 | 7 | 19 | 32 | 27 | 2 | -9 | 2 | 20 | 22 | 19 | 2 | -3 | 8 | 20 | 16 | 10 | 4 | -3 | 8 | 21 | 0 | 3 | 1 |
| -8 | 2 | 19 | 30 | 32 | 1 | -6 | 7 | 19 | 48 | 44 | 1 | -8 | 2 | 20 | 24 | 22 | 1 | -2 | 8 | 20 | 0 | 7 | 1 | -8 | 0 | 22 | 0 | 0 | 1 |
| -7 | 2 | 19 | 26 | 27 | 2 | -5 | 7 | 19 | 25 | 27 | 4 | -7 | 2 | 20 | 83 | 79 | 1 | -1 | 8 | 20 | 23 | 23 | 1 | -7 | 0 | 22 | 18 | 14 | 4 |
| -6 | 2 | 19 | 15 | 15 | 2 | -4 | 7 | 19 | 67 | 60 | 2 | -6 | 2 | 20 | 61 | 59 | 1 | -6 | 9 | 20 | 13 | 5 | 6 | -6 | 0 | 22 | 81 | 76 | 1 |
| -5 | 2 | 19 | 27 | 31 | 1 | -3 | 7 | 19 | 18 | 15 | 2 | -5 | 2 | 20 | 13 | 0 | 6 | -5 | 9 | 20 | 24 | 9 | 4 | -5 | 0 | 22 | 28 | 30 | 3 |
| -4 | 2 | 19 | 0 | 6 | 1 | -2 | 7 | 19 | 77 | 75 | 1 | -4 | 2 | 20 | 14 | 1 | 8 | -4 | 9 | 20 | 53 | 54 | 1 | -4 | 0 | 22 | 44 | 44 | 1 |
| -3 | 2 | 19 | 82 | 79 | 1 | -1 | 7 | 19 | 45 | 44 | 1 | -3 | 2 | 20 | 0 | 12 | 1 | -2 | 9 | 20 | 21 | 15 | 3 | -3 | 0 | 22 | 0 | 20 | 1 |
| -2 | 2 | 19 | 8 | 4 | 8 | 0 | 7 | 19 | 17 | 7 | 2 | -2 | 2 | 20 | 39 | 43 | 1 | -4 | 10 | 20 | 27 | 21 | 4 | -2 | 0 | 22 | 0 | 19 | 1 |
| -1 | 2 | 19 | 26 | 24 | 3 | 1 | 7 | 19 | 13 | 16 | 4 | -1 | 2 | 20 | 39 | 41 | 1 | -9 | 1 | 21 | 0 | 3 | 1 | -1 | 0 | 22 | 17 | 17 | 5 |
| 0 | 2 | 19 | 21 | 18 | 2 | -9 | 8 | 19 | 0 | 6 | 1 | 0 | 2 | 20 | 47 | 46 | 1 | -8 | 1 | 21 | 11 | 6 | 8 | -8 | 1 | 22 | 10 | 6 | 10 |
| 1 | 2 | 19 | 14 | 8 | 4 | -8 | 8 | 19 | 0 | 0 | 1 | 1 | 2 | 20 | 38 | 42 | 1 | -7 | 1 | 21 | 81 | 80 | 1 | -7 | 1 | 22 | 15 | 2 | 3 |
| 2 | 2 | 19 | 11 | 8 | 11 | -7 | 8 | 19 | 14 | 0 | 3 | 2 | 2 | 20 | 0 | 2 | 1 | -6 | 1 | 21 | 39 | 43 | 1 | -6 | 1 | 22 | 13 | 8 | 7 |
| 3 | 2 | 19 | 51 | 54 | 1 | -6 | 8 | 19 | 23 | 18 | 2 | -10 | 3 | 20 | 12 | 5 | 12 | -5 | 1 | 21 | 44 | 49 | 1 | -5 | 1 | 22 | 32 | 26 | 3 |
| -10 | 3 | 19 | 13 | 9 | 4 | -5 | 8 | 19 | 43 | 42 | 1 | -9 | 3 | 20 | 23 | 26 | 2 | -4 | 1 | 21 | 46 | 44 | 2 | -4 | 1 | 22 | 24 | 22 | 2 |
| -9 | 3 | 19 | 9 | 3 | 8 | -4 | 8 | 19 | 10 | 8 | 10 | -8 | 3 | 20 | 19 | 12 | 2 | -3 | 1 | 21 | 52 | 57 | 1 | -3 | 1 | 22 | 0 | 8 | 1 |
| -8 | 3 | 19 | 19 | 13 | 2 | -3 | 8 | 19 | 36 | 34 | 1 | -7 | 3 | 20 | 35 | 40 | 1 | -2 | 1 | 21 | 70 | 64 | 1 | -2 | 1 | 22 | 16 | 16 | 5 |
| -7 | 3 | 19 | 24 | 20 | 2 | -2 | 8 | 19 | 68 | 71 | 5 | -6 | 3 | 20 | 11 | 11 | 4 | -1 | 1 | 21 | 24 | 25 | 2 | -1 | 1 | 22 | 0 | 10 | 1 |
| -6 | 3 | 19 | 58 | 60 | 3 | -1 | 8 | 19 | 14 | 6 | 2 | -5 | 3 | 20 | 13 | 13 | 2 | 0 | 1 | 21 | 61 | 57 | 1 | -7 | 2 | 22 | 19 | 15 | 3 |
| -5 | 3 | 19 | 7 | 7 | 6 | 0 | 8 | 19 | 20 | 22 | 2 | -4 | 3 | 20 | 57 | 59 | 1 | -9 | 2 | 21 | 12 | 13 | 7 | -6 | 2 | 22 | 0 | 3 | 1 |
| -4 | 3 | 19 | 13 | 4 | 4 | 1 | 8 | 19 | 21 | 17 | 4 | -3 | 3 | 20 | 9 | 4 | 8 | -8 | 2 | 21 | 26 | 17 | 4 | -5 | 2 | 22 | 10 | 8 | 9 |
| -3 | 3 | 19 | 32 | 33 | 1 | -8 | 9 | 19 | 8 | 3 | 8 | -2 | 3 | 20 | 43 | 42 | 1 | -7 | 2 | 21 | 30 | 29 | 1 | -4 | 2 | 22 | 19 | 19 | 3 |
| -2 | 3 | 19 | 0 | 5 | 1 | -7 | 9 | 19 | 26 | 25 | 4 | -1 | 3 | 20 | 14 | 15 | 4 | -6 | 2 | 21 | 43 | 48 | 3 | -3 | 2 | 22 | 18 | 8 | 6 |
| -1 | 3 | 19 | 26 | 31 | 3 | -6 | 9 | 19 | 25 | 17 | 2 | 0 | 3 | 20 | 12 | 11 | 10 | -5 | 2 | 21 | 50 | 47 | 1 | -2 | 2 | 22 | 23 | 21 | 2 |
| 0 | 3 | 19 | 24 | 20 | 2 | -5 | 9 | 19 | 18 | 6 | 2 | 1 | 3 | 20 | 23 | 29 | 3 | -4 | 2 | 21 | 63 | 56 | 1 | -1 | 2 | 22 | 25 | 23 | 4 |
| 1 | 3 | 19 | 19 | 9 | 2 | -4 | 9 | 19 | 19 | 13 | 3 | -9 | 4 | 20 | 0 | 1 | 1 | -3 | 2 | 21 | 60 | 54 | 2 | -7 | 3 | 22 | 17 | 16 | 5 |
| 2 | 3 | 19 | 14 | 9 | 5 | -3 | 9 | 19 | 19 | 3 | 3 | -8 | 4 | 20 | 0 | 0 | 1 | -2 | 2 | 21 | 15 | 0 | 4 | -6 | 3 | 22 | 22 | 24 | 2 |
| 3 | 3 | 19 | 7 | 4 | 7 | -2 | 9 | 19 | 0 | 19 | 1 | -7 | 4 | 20 | 14 | 11 | 5 | -1 | 2 | 21 | 16 | 14 | 3 | -5 | 3 | 22 | 24 | 26 | 4 |
| -10 | 4 | 19 | 54 | 53 | 1 | -1 | 9 | 19 | 26 | 16 | 3 | -6 | 4 | 20 | 20 | 14 | 2 | 0 | 2 | 21 | 22 | 32 | 4 | -4 | 3 | 22 | 16 | 25 | 6 |
| -9 | 4 | 19 | 15 | 6 | 4 | 0 | 9 | 19 | 31 | 31 | 2 | -5 | 4 | 20 | 25 | 33 | 1 | -9 | 3 | 21 | 17 | 15 | 4 | -3 | 3 | 22 | 45 | 40 | 3 |
| -8 | 4 | 19 | 38 | 39 | 2 | -7 | 10 | 19 | 33 | 30 | 4 | -4 | 4 | 20 | 40 | 43 | 1 | -8 | 3 | 21 | 25 | 21 | 2 | -7 | 4 | 22 | 11 | 12 | 11 |
| -7 | 4 | 19 | 11 | 4 | 7 | -6 | 10 | 19 | 22 | 24 | 4 | -3 | 4 | 20 | 45 | 51 | 3 | -7 | 3 | 21 | 31 | 34 | 2 | -6 | 4 | 22 | 15 | 12 | 8 |
| -6 | 4 | 19 | 47 | 49 | 1 | | | | | | | | | | | | | | | | | | | | | | | | |

Anexo 3.

Rayos-X de exo,exo-105

R-X de *exo,exo*-105.

PCHC17a

Experimental. A prismatic crystal (0.1x0.1x0.2 mm) was selected and mounted on a Enraf-Nonius CAD4 four-circle diffractometer. Unit-cell parameters were determined from automatic centering of 25 reflections ($12 < \theta < 21^\circ$) and refined by least-squares method. Intensities were collected with graphite monochromatized Mo K α radiation, using $\omega/2\theta$ scan-technique. 2349 reflections were measured in the range $2.25 \leq \theta \leq 30.08$. 707 reflections were assumed as observed applying the condition $I > 2\sigma(I)$. Three reflections were measured every two hours as orientation and intensity control, significant intensity decay was not observed. Lorentz-polarization but no absorption corrections were made.

The structure was solved by Direct methods, using SHELXS computer program (Sheldrick, G.M., (1997), A computer program for determination of crystal structure. Univer Göttingen, Germany) and refined by full-matrix least-squares method with SHELX97 computer program (Sheldrick, G.M., (1997), A computer program for determination of crystal structure. Univer Göttingen, Germany), using 2349 reflections, (very negative intensities were not assumed). The function minimized was $\sum w ||F_o|^2 - |F_c|^2|^2$, where $w = [\sigma^2(I) + (0.1041 P)^2]^{-1}$, and $P = (|F_o|^2 + 2|F_c|^2)/3$, f , f' and f'' were taken from International Tables of X-Ray Crystallography (International Tables of X-Ray Crystallography, (1974), Ed. Kynoch press, Vol. IV, pp 99-100 and 149). The chirality of structure was define from the Flack coefficient, which it is equal to $\bar{6}(4)$ for the given results (Flack, H.D., (1983), Acta Cryst., A39, 876-881). All H atoms were computed and refined, using a riding model, with an isotropic temperature factor equal to 1.2 time the equivalent temperature factor of the atom which are linked. The final R(on F) factor was 0.049, $wR(on |F|^2) = 0.140$ and goodness of fit = 0.817 for all observed reflections. Number of refined parameters was 127. Max. shift/esd = 0.00, Mean shift/esd = 0.00. Max. and min. peaks in final difference synthesis was 0.169 and -0.162 e \AA^{-3} , respectively.

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Table 1. Crystal data and structure refinement for pchcl7a.

| | |
|-----------------------------------|---|
| Identification code | pchcl7a |
| Empirical formula | C ₂₄ H ₂₄ O ₄ |
| Formula weight | 376.43 |
| Temperature | 293(2) K |
| Wavelength | 0.71069 Å |
| Crystal system, space group | Orthorhombic, Fdd2 |
| Unit cell dimensions | a = 16.161(9) Å α = 90 °. b = 17.821(16) Å β = 90 °. c = 13.764(9) Å γ = 90 °. |
| Volume | 3964(5) Å ³ |
| Z, Calculated density | 8, 1.261 Mg/m ³ |
| Absorption coefficient | 0.085 mm ⁻¹ |
| F(000) | 1600 |
| Crystal size | 0.1 x 0.1 x 0.2 mm |
| Theta range for data collection | 2.25 to 30.08 °. |
| Index ranges | 0<=h<=22, 0<=k<=25, -19<=l<=15 |
| Reflections collected / unique | 2349 / 2349 [R(int) = 0.0386] |
| Refinement method | Full-matrix least-squares on F ² |
| Data / restraints / parameters | 2349 / 1 / 127 |
| Goodness-of-fit on F ² | 0.817 |
| Final R indices [I>2σ(I)] | R1 = 0.0495, wR2 = 0.1401 |
| R indices (all data) | R1 = 0.1928, wR2 = 0.1986 |
| Largest diff. peak and hole | 0.169 and -0.162 e.Å ⁻³ |

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for pchcl7a. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|---------|----------|--------|
| O(1) | -1467(5) | 1816(4) | 3208(5) | 209(3) |
| O(2) | -777(3) | 1894(3) | 4423(5) | 173(2) |
| C(1) | 1619(3) | 618(2) | 1328(3) | 82(1) |
| C(2) | 2031(3) | 737(3) | 456(4) | 101(1) |
| C(3) | 1626(4) | 526(3) | -404(4) | 107(2) |
| C(4) | 847(4) | 227(3) | -370(3) | 96(1) |
| C(5) | 437(2) | 152(2) | 507(3) | 70(1) |
| C(6) | 823(2) | 333(2) | 1373(3) | 65(1) |
| C(7) | 414(2) | 225(2) | 2346(3) | 61(1) |
| C(8) | 172(2) | 1002(2) | 2751(3) | 74(1) |
| C(9) | -493(3) | 817(2) | 3513(4) | 94(1) |
| C(10) | -987(2) | 205(2) | 3073(3) | 76(1) |
| C(11) | -993(4) | 1528(4) | 3725(5) | 115(2) |
| C(12) | -1279(7) | 2659(5) | 4334(10) | 273(8) |

Table 3. Bond lengths [Å] and angles [°] for pchc17a.

| | |
|---------------------|----------|
| O(1)-C(11) | 1.164(7) |
| O(2)-C(11) | 1.213(7) |
| O(2)-C(12) | 1.592(9) |
| C(1)-C(6) | 1.385(5) |
| C(1)-C(2) | 1.388(6) |
| C(2)-C(3) | 1.404(7) |
| C(3)-C(4) | 1.367(7) |
| C(4)-C(5) | 1.383(6) |
| C(5)-C(6) | 1.383(5) |
| C(5)-C(5)#1 | 1.514(8) |
| C(6)-C(7) | 1.506(5) |
| C(7)-C(8) | 1.543(5) |
| C(7)-C(7)#1 | 1.560(7) |
| C(7)-C(10)#1 | 1.564(5) |
| C(8)-C(9) | 1.538(6) |
| C(9)-C(10) | 1.481(6) |
| C(9)-C(11) | 1.530(8) |
| C(10)-C(7)#1 | 1.564(5) |
| <hr/> | |
| C(11)-O(2)-C(12) | 104.7(7) |
| C(6)-C(1)-C(2) | 122.6(5) |
| C(1)-C(2)-C(3) | 117.7(5) |
| C(4)-C(3)-C(2) | 120.3(5) |
| C(3)-C(4)-C(5) | 120.5(5) |
| C(4)-C(5)-C(6) | 120.9(4) |
| C(4)-C(5)-C(5)#1 | 118.8(3) |
| C(6)-C(5)-C(5)#1 | 120.3(2) |
| C(5)-C(6)-C(1) | 117.8(4) |
| C(5)-C(6)-C(7) | 122.6(3) |
| C(1)-C(6)-C(7) | 119.6(4) |
| C(6)-C(7)-C(8) | 108.5(3) |
| C(6)-C(7)-C(7)#1 | 116.2(2) |
| C(8)-C(7)-C(7)#1 | 104.1(3) |
| C(6)-C(7)-C(10)#1 | 111.8(3) |
| C(8)-C(7)-C(10)#1 | 111.1(3) |
| C(7)#1-C(7)-C(10)#1 | 104.9(3) |
| C(9)-C(8)-C(7) | 103.3(3) |
| C(10)-C(9)-C(11) | 113.8(4) |
| C(10)-C(9)-C(8) | 104.8(3) |
| C(11)-C(9)-C(8) | 108.7(4) |
| C(9)-C(10)-C(7)#1 | 107.6(3) |
| O(1)-C(11)-O(2) | 115.9(7) |
| O(1)-C(11)-C(9) | 126.6(7) |
| O(2)-C(11)-C(9) | 116.4(7) |

Symmetry transformations used to generate equivalent atoms:
#1 -x, -y, z

Table 4. Hydrogen bond lengths [Å] and angles [°] for pchcl7a.

| | |
|---------------------|--------|
| C(1)-H(1) | 0.9300 |
| C(2)-H(2) | 0.9300 |
| C(3)-H(3) | 0.9300 |
| C(4)-H(4) | 0.9300 |
| C(8)-H(8) | 0.9700 |
| C(8)-H(8A) | 0.9700 |
| C(9)-H(9) | 0.9800 |
| C(10)-H(10) | 0.9700 |
| C(10)-H(10A) | 0.9700 |
| C(12)-H(12) | 0.9600 |
| C(12)-H(12A) | 0.9600 |
| C(12)-H(12B) | 0.9600 |
| | |
| C(6)-C(1)-H(1) | 118.7 |
| C(2)-C(1)-H(1) | 118.7 |
| C(1)-C(2)-H(2) | 121.1 |
| C(3)-C(2)-H(2) | 121.1 |
| C(4)-C(3)-H(3) | 119.9 |
| C(2)-C(3)-H(3) | 119.9 |
| C(3)-C(4)-H(4) | 119.7 |
| C(5)-C(4)-H(4) | 119.7 |
| C(9)-C(8)-H(8) | 111.1 |
| C(7)-C(8)-H(8) | 111.1 |
| C(9)-C(8)-H(8A) | 111.1 |
| C(7)-C(8)-H(8A) | 111.1 |
| H(8)-C(8)-H(8A) | 109.1 |
| C(10)-C(9)-H(9) | 109.8 |
| C(11)-C(9)-H(9) | 109.8 |
| C(8)-C(9)-H(9) | 109.8 |
| C(9)-C(10)-H(10) | 110.2 |
| C(7)#1-C(10)-H(10) | 110.2 |
| C(9)-C(10)-H(10A) | 110.2 |
| C(7)#1-C(10)-H(10A) | 110.2 |
| H(10)-C(10)-H(10A) | 108.5 |
| O(2)-C(12)-H(12) | 109.5 |
| O(2)-C(12)-H(12A) | 109.5 |
| H(12)-C(12)-H(12A) | 109.5 |
| O(2)-C(12)-H(12B) | 109.5 |
| H(12)-C(12)-H(12B) | 109.5 |
| H(12A)-C(12)-H(12B) | 109.5 |

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for pchcl7a.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

| | U_{11} | U_{22} | U_{33} | U_{23} | U_{13} | U_{12} |
|-------|----------|----------|----------|----------|----------|----------|
| O(1) | 241(7) | 236(7) | 150(5) | -13(4) | 8(5) | 98(6) |
| O(2) | 157(4) | 189(5) | 175(4) | -49(4) | 1(4) | 21(4) |
| C(1) | 82(3) | 75(2) | 89(3) | 0(2) | 13(3) | -2(2) |
| C(2) | 93(3) | 100(3) | 111(4) | 6(3) | 14(4) | 1(2) |
| C(3) | 131(5) | 112(4) | 79(4) | 13(3) | 19(3) | 10(4) |
| C(4) | 109(4) | 105(4) | 74(4) | 3(3) | 0(3) | -3(3) |
| C(5) | 78(2) | 57(2) | 74(3) | -1(2) | 2(2) | 6(2) |
| C(6) | 69(2) | 53(2) | 73(3) | -2(2) | 4(2) | 2(2) |
| C(7) | 63(2) | 57(2) | 64(2) | 2(2) | 5(2) | 3(2) |
| C(8) | 82(3) | 66(2) | 74(3) | -3(2) | 3(2) | -3(2) |
| C(9) | 95(3) | 93(3) | 94(3) | -13(2) | 3(3) | 2(3) |
| C(10) | 72(2) | 80(2) | 76(3) | -1(2) | 3(2) | -2(2) |
| C(11) | 103(4) | 125(5) | 118(5) | -50(4) | 26(4) | 1(3) |
| C(12) | 256(12) | 158(7) | 200(2) | -18(10) | 75(13) | 58(7) |

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for pchcl7a.

| | x | y | z | U(eq) |
|--------|-------|------|------|-------|
| H(1) | 1889 | 735 | 1905 | 98 |
| H(2) | 2556 | 949 | 442 | 121 |
| H(3) | 1889 | 589 | -999 | 129 |
| H(4) | 591 | 73 | -941 | 115 |
| H(8) | 644 | 1249 | 3047 | 89 |
| H(8A) | -49 | 1322 | 2243 | 89 |
| H(9) | -230 | 638 | 4111 | 113 |
| H(10) | -1462 | 411 | 2733 | 91 |
| H(10A) | -1186 | -133 | 3573 | 91 |
| H(12) | -1112 | 2994 | 4844 | 327 |
| H(12A) | -1861 | 2559 | 4390 | 327 |
| H(12B) | -1167 | 2886 | 3716 | 327 |

Table 8. Torsion angles [°] for pchcl7a.

| | |
|-------------------------|-----------|
| C(6)-C(1)-C(2)-C(3) | -2.8(6) |
| C(1)-C(2)-C(3)-C(4) | 1.1(7) |
| C(2)-C(3)-C(4)-C(5) | 2.2(7) |
| C(3)-C(4)-C(5)-C(6) | -4.1(6) |
| C(3)-C(4)-C(5)-C(5)#1 | 177.5(4) |
| C(4)-C(5)-C(6)-C(1) | 2.4(5) |
| C(5)#1-C(5)-C(6)-C(1) | -179.2(4) |
| C(4)-C(5)-C(6)-C(7) | -177.0(4) |
| C(5)#1-C(5)-C(6)-C(7) | 1.4(5) |
| C(2)-C(1)-C(6)-C(5) | 1.0(5) |
| C(2)-C(1)-C(6)-C(7) | -179.6(4) |
| C(5)-C(6)-C(7)-C(8) | -107.1(4) |
| C(1)-C(6)-C(7)-C(8) | 73.5(4) |
| C(5)-C(6)-C(7)-C(7)#1 | 9.7(5) |
| C(1)-C(6)-C(7)-C(7)#1 | -169.7(3) |
| C(5)-C(6)-C(7)-C(10)#1 | 130.1(4) |
| C(1)-C(6)-C(7)-C(10)#1 | -49.3(4) |
| C(6)-C(7)-C(8)-C(9) | 160.1(3) |
| C(7)#1-C(7)-C(8)-C(9) | 35.7(3) |
| C(10)#1-C(7)-C(8)-C(9) | -76.7(4) |
| C(7)-C(8)-C(9)-C(10) | -39.0(4) |
| C(7)-C(8)-C(9)-C(11) | -161.0(4) |
| C(11)-C(9)-C(10)-C(7)#1 | 145.4(4) |
| C(8)-C(9)-C(10)-C(7)#1 | 26.7(4) |
| C(12)-O(2)-C(11)-O(1) | 0.7(9) |
| C(12)-O(2)-C(11)-C(9) | 169.1(6) |
| C(10)-C(9)-C(11)-O(1) | -45.0(9) |
| C(8)-C(9)-C(11)-O(1) | 71.4(8) |
| C(10)-C(9)-C(11)-O(2) | 148.1(6) |
| C(8)-C(9)-C(11)-O(2) | -95.5(7) |

Symmetry transformations used to generate equivalent atoms:

#1 -x, -y, z

Analysis of Potential Hydrogen Bonds

| Typ | Donor | --- | H... | Acceptor | [| ARU |] | D - H | H...A | D...A | D - H...A |
|-------|-------|-----|-------|----------|------|-----|---|--------|--------|----------|-----------|
| Intra | C(10) | -- | H(10) | .. | O(1) | [|] | 0.9711 | 2.5878 | 2.980(8) | 104.27 |

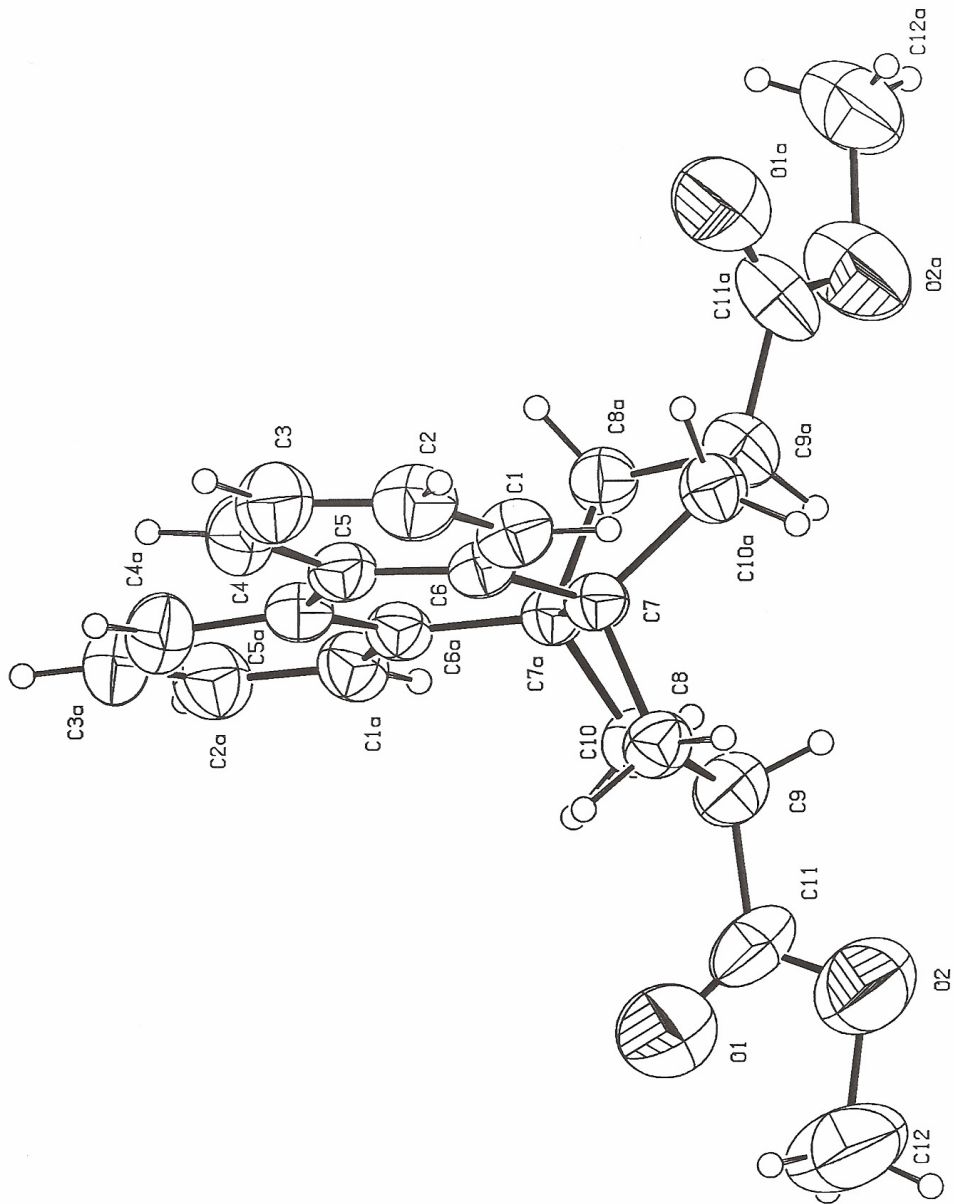


Table 10. Observed and calculated structure factors for pchcl7a

Page 1

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|----|-------|-----|------|------|-----|-------|----|----|------|------|-------|-----|-----|----|------|-------|-----|-----|----|----|-------|------|-----|-----|---|---|------|------|-----|
| 1 | 1-19 | 39 | 13 | 39 | 7 | 1-15 | 0 | 39 | 1 | 10 | 12-14 | 0 | 21 | 1 | 12 | 4-12 | 37 | 34 | 36 | 3 | 9-11 | 250 | 256 | 9 | | | | | |
| 3 | 1-19 | 34 | 8 | 33 | 9 | 1-15 | 16 | 5 | 15 | 0 | 14-14 | 0 | 20 | 1 | 14 | 4-12 | 64 | 43 | 59 | 5 | 9-11 | 195 | 200 | 7 | | | | | |
| 1 | 3-19 | 42 | 4 | 41 | 11 | 1-15 | 58 | 15 | 58 | 2 | 14-14 | 100 | 20 | 34 | 16 | 4-12 | 0 | 32 | 1 | 7 | 9-11 | 78 | 92 | 33 | | | | | |
| 3 | 3-19 | 0 | 16 | 1 | 13 | 1-15 | 0 | 33 | 1 | 4 | 14-14 | 0 | 2 | 1 | 2 | 6-12 | 261 | 271 | 10 | 9 | 9-11 | 0 | 33 | 1 | | | | | |
| 1 | 5-19 | 0 | 18 | 1 | 1 | 3-15 | 0 | 53 | 1 | 6 | 14-14 | 0 | 13 | 1 | 4 | 6-12 | 137 | 127 | 11 | 11 | 9-11 | 0 | 24 | 1 | | | | | |
| 2 | 0-18 | 0 | 25 | 1 | 3 | 3-15 | 47 | 41 | 46 | 8 | 14-14 | 0 | 14 | 1 | 6 | 6-12 | 139 | 162 | 10 | 13 | 9-11 | 76 | 56 | 76 | | | | | |
| 0 | 2-18 | 44 | 38 | 44 | 5 | 3-15 | 0 | 30 | 1 | 2 | 16-14 | 38 | 13 | 37 | 8 | 6-12 | 0 | 55 | 1 | 15 | 9-11 | 0 | 19 | 1 | | | | | |
| 6 | 0-18 | 83 | 58 | 82 | 7 | 3-15 | 0 | 23 | 1 | 4 | 16-14 | 46 | 19 | 45 | 10 | 6-12 | 0 | 45 | 1 | 1 | 11-11 | 0 | 87 | 1 | | | | | |
| 2 | 2-18 | 0 | 20 | 1 | 9 | 3-15 | 34 | 4 | 33 | 1 | 1-13 | 139 | 123 | 10 | 12 | 6-12 | 37 | 13 | 36 | 3 | 11-11 | 100 | 100 | 34 | | | | | |
| 4 | 2-18 | 0 | 41 | 1 | 11 | 3-15 | 0 | 21 | 1 | 3 | 1-13 | 0 | 15 | 1 | 14 | 6-12 | 0 | 30 | 1 | 5 | 11-11 | 147 | 136 | 16 | | | | | |
| 6 | 2-18 | 0 | 15 | 1 | 13 | 3-15 | 0 | 46 | 1 | 5 | 1-13 | 58 | 61 | 35 | 16 | 6-12 | 0 | 12 | 1 | 7 | 11-11 | 56 | 21 | 55 | | | | | |
| 8 | 2-18 | 30 | 18 | 29 | 1 | 5-15 | 69 | 94 | 68 | 7 | 1-13 | 0 | 41 | 1 | 0 | 8-12 | 88 | 99 | 87 | 9 | 11-11 | 53 | 22 | 52 | | | | | |
| 2 | 4-18 | 20 | 20 | 20 | 3 | 5-15 | 55 | 57 | 55 | 9 | 1-13 | 0 | 28 | 1 | 2 | 8-12 | 48 | 68 | 48 | 11 | 11-11 | 0 | 50 | 1 | | | | | |
| 4 | 4-18 | 35 | 11 | 35 | 5 | 5-15 | 0 | 40 | 1 | 11 | 1-13 | 29 | 30 | 29 | 4 | 8-12 | 35 | 25 | 34 | 13 | 11-11 | 0 | 38 | 1 | | | | | |
| 6 | 4-18 | 0 | 20 | 1 | 7 | 5-15 | 41 | 30 | 40 | 13 | 1-13 | 33 | 30 | 33 | 6 | 8-12 | 0 | 86 | 1 | 15 | 11-11 | 0 | 16 | 1 | | | | | |
| 0 | 6-18 | 49 | 10 | 48 | 9 | 5-15 | 46 | 4 | 45 | 15 | 1-13 | 0 | 14 | 1 | 8 | 8-12 | 56 | 45 | 55 | 1 | 13-11 | 0 | 68 | 1 | | | | | |
| 2 | 6-18 | 0 | 32 | 1 | 11 | 5-15 | 0 | 31 | 1 | 1 | 3-13 | 135 | 138 | 10 | 10 | 8-12 | 82 | 57 | 25 | 3 | 13-11 | 65 | 71 | 65 | | | | | |
| 4 | 6-18 | 53 | 14 | 52 | 13 | 5-15 | 0 | 18 | 1 | 3 | 3-13 | 0 | 37 | 1 | 12 | 8-12 | 55 | 44 | 54 | 5 | 13-11 | 127 | 125 | 22 | | | | | |
| 6 | 6-18 | 0 | 10 | 1 | 1 | 7-15 | 0 | 54 | 1 | 5 | 3-13 | 77 | 51 | 20 | 14 | 8-12 | 0 | 18 | 1 | 7 | 13-11 | 0 | 32 | 1 | | | | | |
| 2 | 8-18 | 27 | 11 | 27 | 3 | 7-15 | 0 | 26 | 1 | 7 | 3-13 | 27 | 25 | 26 | 16 | 8-12 | 17 | 13 | 17 | 9 | 13-11 | 0 | 14 | 1 | | | | | |
| 4 | 8-18 | 62 | 26 | 62 | 5 | 7-15 | 0 | 26 | 1 | 9 | 3-13 | 45 | 45 | 44 | 2 | 10-12 | 48 | 57 | 47 | 11 | 13-11 | 27 | 17 | 27 | | | | | |
| 1 | 1-17 | 0 | 31 | 1 | 7 | 7-15 | 0 | 48 | 1 | 11 | 3-13 | 0 | 14 | 1 | 4 | 10-12 | 141 | 132 | 11 | 13 | 13-11 | 28 | 30 | 27 | | | | | |
| 3 | 1-17 | 63 | 58 | 63 | 9 | 7-15 | 0 | 61 | 1 | 13 | 3-13 | 0 | 41 | 1 | 6 | 10-12 | 0 | 28 | 1 | 1 | 15-11 | 0 | 23 | 1 | | | | | |
| 5 | 1-17 | 0 | 49 | 1 | 11 | 7-15 | 0 | 14 | 1 | 15 | 3-13 | 54 | 45 | 53 | 8 | 10-12 | 0 | 66 | 1 | 3 | 15-11 | 66 | 66 | 65 | | | | | |
| 7 | 1-17 | 44 | 16 | 43 | 13 | 7-15 | 0 | 11 | 1 | 1 | 5-13 | 54 | 51 | 53 | 10 | 10-12 | 28 | 23 | 28 | 5 | 15-11 | 111 | 97 | 111 | | | | | |
| 9 | 1-17 | 0 | 22 | 1 | 1 | 9-15 | 40 | 27 | 40 | 3 | 5-13 | 80 | 88 | 69 | 12 | 10-12 | 0 | 24 | 1 | 7 | 15-11 | 70 | 75 | 70 | | | | | |
| 1 | 3-17 | 0 | 20 | 1 | 3 | 9-15 | 0 | 27 | 1 | 5 | 5-13 | 47 | 39 | 47 | 14 | 10-12 | 68 | 13 | 45 | 9 | 15-11 | 0 | 18 | 1 | | | | | |
| 3 | 3-17 | 70 | 35 | 70 | 5 | 9-15 | 0 | 28 | 1 | 7 | 5-13 | 54 | 61 | 54 | 0 | 12-12 | 84 | 77 | 56 | 11 | 15-11 | 0 | 20 | 1 | | | | | |
| 5 | 3-17 | 0 | 42 | 1 | 7 | 9-15 | 53 | 48 | 52 | 9 | 5-13 | 51 | 46 | 50 | 2 | 12-12 | 0 | 14 | 1 | 1 | 17-11 | 37 | 41 | 37 | | | | | |
| 7 | 3-17 | 39 | 7 | 38 | 9 | 9-15 | 0 | 40 | 1 | 11 | 5-13 | 29 | 18 | 28 | 4 | 12-12 | 0 | 41 | 1 | 3 | 17-11 | 0 | 24 | 1 | | | | | |
| 9 | 3-17 | 0 | 14 | 1 | 11 | 9-15 | 0 | 9 | 1 | 13 | 5-13 | 66 | 39 | 66 | 6 | 12-12 | 0 | 62 | 1 | 5 | 17-11 | 46 | 45 | 45 | | | | | |
| 1 | 5-17 | 45 | 56 | 45 | 1 | 11-15 | 0 | 14 | 1 | 15 | 5-13 | 0 | 30 | 1 | 8 | 12-12 | 0 | 12 | 1 | 7 | 17-11 | 70 | 65 | 69 | | | | | |
| 3 | 5-17 | 0 | 5 | 1 | 3 | 11-15 | 0 | 5 | 1 | 1 | 7-13 | 91 | 111 | 26 | 10 | 12-12 | 0 | 10 | 1 | 9 | 17-11 | 78 | 51 | 78 | | | | | |
| 5 | 5-17 | 45 | 25 | 45 | 5 | 11-15 | 0 | 19 | 1 | 3 | 7-13 | 63 | 42 | 42 | 12 | 12-12 | 0 | 28 | 1 | 1 | 19-11 | 0 | 50 | 1 | | | | | |
| 7 | 5-17 | 0 | 10 | 1 | 5 | 11-15 | 51 | 37 | 51 | 5 | 7-13 | 66 | 74 | 65 | 14 | 12-12 | 0 | 25 | 1 | 3 | 19-11 | 34 | 36 | 33 | | | | | |
| 9 | 5-17 | 0 | 14 | 1 | 7 | 11-15 | 51 | 26 | 56 | 7 | 7-13 | 40 | 35 | 39 | 2 | 14-12 | 79 | 30 | 65 | 5 | 19-11 | 0 | 30 | 1 | | | | | |
| 1 | 7-17 | 0 | 4 | 1 | 1 | 13-15 | 0 | 14 | 1 | 9 | 7-13 | 0 | 42 | 1 | 4 | 14-12 | 69 | 80 | 68 | 2 | 0-10 | 254 | 239 | 6 | | | | | |
| 3 | 7-17 | 47 | 11 | 47 | 3 | 13-15 | 47 | 11 | 47 | 11 | 7-13 | 42 | 39 | 42 | 6 | 14-12 | 62 | 67 | 62 | 6 | 0-10 | 59 | 45 | 58 | | | | | |
| 5 | 7-17 | 0 | 18 | 1 | 5 | 13-15 | 32 | 20 | 32 | 13 | 7-13 | 66 | 14 | 53 | 8 | 14-12 | 0 | 31 | 1 | 10 | 0-10 | 215 | 207 | 10 | | | | | |
| 7 | 7-17 | 61 | 43 | 61 | 7 | 13-15 | 50 | 21 | 50 | 15 | 7-13 | 0 | 18 | 1 | 10 | 14-12 | 0 | 15 | 1 | 14 | 0-10 | 63 | 17 | 63 | | | | | |
| 9 | 7-17 | 74 | 45 | 73 | 1 | 15-15 | 0 | 18 | 1 | 1 | 9-13 | 0 | 31 | 1 | 12 | 14-12 | 40 | 17 | 40 | 18 | 0-10 | 0 | 9 | 1 | | | | | |
| 1 | 9-17 | 0 | 31 | 1 | 3 | 15-15 | 0 | 9 | 1 | 3 | 9-13 | 72 | 103 | 56 | 0 | 16-12 | 43 | 17 | 43 | 0 | 2-10 | 495 | 513 | 4 | | | | | |
| 3 | 9-17 | 0 | 9 | 1 | 2 | 0-14 | 58 | 58 | 58 | 5 | 9-13 | 63 | 60 | 62 | 2 | 16-12 | 76 | 12 | 76 | 2 | 2-10 | 173 | 145 | 5 | | | | | |
| 5 | 9-17 | 0 | 31 | 1 | 6 | 0-14 | 0 | 73 | 1 | 7 | 9-13 | 0 | 42 | 1 | 4 | 16-12 | 0 | 23 | 1 | 4 | 2-10 | 123 | 77 | 11 | | | | | |
| 7 | 9-17 | 0 | 18 | 1 | 10 | 0-14 | 0 | 23 | 1 | 9 | 9-13 | 59 | 47 | 59 | 6 | 16-12 | 62 | 74 | 62 | 6 | 2-10 | 62 | 49 | 22 | | | | | |
| 1 | 11-17 | 0 | 25 | 1 | 14 | 0-14 | 0 | 37 | 1 | 11 | 9-13 | 28 | 43 | 27 | 8 | 16-12 | 0 | 25 | 1 | 8 | 2-10 | 236 | 226 | 6 | | | | | |
| 3 | 11-17 | 0 | 7 | 1 | 0 | 2-14 | 58 | 54 | 57 | 13 | 9-13 | 60 | 23 | 59 | 10 | 16-12 | 0 | 26 | 1 | 10 | 2-10 | 75 | 78 | 25 | | | | | |
| 0 | 0-16 | 0 | 8 | 1 | 2 | 2-14 | 0 | 62 | 1 | 1 | 11-13 | 33 | 41 | 33 | 2 | 18-12 | 0 | 38 | 1 | 12 | 2-10 | 0 | 44 | 1 | | | | | |
| 4 | 0-16 | 0 | 78 | 1 | 4 | 2-14 | 49 | 39 | 48 | 3 | 11-13 | 70 | 100 | 38 | 4 | 18-12 | 0 | 15 | 1 | 14 | 2-10 | 71 | 44 | 45 | | | | | |
| 8 | 0-16 | 0 | 17 | 1 | 6 | 2-14 | 0 | 17 | 1 | 5 | 11-13 | 0 | 53 | 1 | 6 | 18-12 | 32 | 41 | 31 | 16 | 2-10 | 0 | 45 | 1 | | | | | |
| 12 | 0-16 | 116 | 79 | 32 | 8 | 2-14 | 0 | 33 | 1 | 7 | 11-13 | 0 | 52 | 1 | 1 | 1-11 | 349 | 353 | 4 | 18 | 2-10 | 0 | 32 | 1 | | | | | |
| 4 | 2-16 | 0 | 50 | 1 | 10 | 2-14 | 0 | 5 | 1 | 9 | 11-13 | 38 | 26 | 37 | 3 | 1-11 | 142 | 154 | 8 | 2 | 4-10 | 325 | 309 | 5 | | | | | |
| 6 | 2-16 | 0 | 8 | 1 | 12 | 2-14 | 55 | 18 | 55 | 11 | 11-13 | 0 | 25 | 1 | 5 | 1-11 | 66 | 85 | 31 | 4 | 4-10 | 37 | 50 | 36 | | | | | |
| 8 | 2-16 | 0 | 15 | 1 | 14 | 2-14 | 0 | 40 | 1 | 13 | 11-13 | 28 | 14 | 28 | 7 | 1-11 | 154 | 149 | 10 | 6 | 4-10 | 75 | 47 | 29 | | | | | |
| 10 | 2-16 | 0 | 11 | 1 | 2 | 4-14 | 60 | 72 | 51 | 1 | 13-13 | 0 | 12 | 1 | 9 | 1-11 | 155 | 158 | 17 | 8 | 4-10 | 108 | 112 | 22 | | | | | |
| 12 | 2-16 | 40 | 34 | 39 | 4 | 4-14 | 54 | 35 | 54 | 3 | 13-13 | 9 | 16 | 9 | 11 | 1-11 | 0 | 34 | 1 | 10 | 4-10 | 86 | 108 | 29 | | | | | |
| 0 | 4-16 | 65 | 57 | 65 | 8 | 4-14 | 34 | 39 | 33 | 5 | 13-13 | 0 | 35 | 1 | 13 | 1-11 | 0 | 29 | 1 | 12 | 4-10 | 80 | 79 | 42 | | | | | |
| 2 | 4-16 | 0 | 50 | 1 | 10 | 4-14 | 0 | 15 | 1 | 9 | 13-13 | 0 | 10 | 1 | 17 | 1-11 | 0 | 28 | 1 | 16 | 4-10 | 0 | 8 | 1 | | | | | |
| 4 | 4-16 | 42 | 52 | 42 | 12 | 4-14 | 0 | 24 | 1 | 11 | 13-13 | 73 | 23 | 73 | 1 | 3-11 | 428 | 429 | 4 | | | | | | | | | | |

Table 10. Observed and calculated structure factors for pch17a

| Observed | | | | calculated | | | | structure factors | | | | for pch17a | | | | | | | |
|----------|-------|-----|------|------------|-----|-------|----|-------------------|------|------|-------|------------|-----|----|------|-------|-----|-----|----|
| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | | |
| 1 | 1-19 | 39 | 13 | 39 | 7 | 1-15 | 0 | 39 | 1 | 10 | 12-14 | 0 | 21 | 1 | 12 | 4-12 | 37 | 34 | 36 |
| 3 | 1-19 | 34 | 8 | 33 | 9 | 1-15 | 16 | 5 | 15 | 0 | 14-14 | 0 | 20 | 1 | 14 | 4-12 | 64 | 43 | 59 |
| 1 | 3-19 | 42 | 4 | 41 | 11 | 1-15 | 58 | 15 | 58 | 2 | 14-14 | 100 | 20 | 34 | 16 | 4-12 | 0 | 32 | 1 |
| 3 | 3-19 | 0 | 16 | 1 | 13 | 1-15 | 0 | 23 | 1 | 4 | 14-14 | 0 | 2 | 1 | 2 | 6-12 | 261 | 271 | 10 |
| 1 | 5-19 | 0 | 18 | 1 | 1 | 3-15 | 0 | 55 | 1 | 6 | 14-14 | 0 | 13 | 1 | 4 | 6-12 | 137 | 127 | 11 |
| 2 | 0-18 | 0 | 25 | 1 | 3 | 3-15 | 47 | 41 | 46 | 8 | 14-14 | 0 | 14 | 1 | 6 | 6-12 | 139 | 162 | 10 |
| 0 | 0-18 | 44 | 38 | 44 | 5 | 3-15 | 0 | 30 | 1 | 2 | 16-14 | 38 | 13 | 37 | 8 | 6-12 | 0 | 55 | 1 |
| 6 | 2-18 | 83 | 58 | 82 | 7 | 3-15 | 0 | 23 | 1 | 4 | 16-14 | 46 | 19 | 45 | 10 | 6-12 | 0 | 45 | 1 |
| 2 | 2-18 | 0 | 20 | 1 | 9 | 3-15 | 34 | 4 | 33 | 1 | 1-13 | 139 | 123 | 10 | 12 | 6-12 | 37 | 13 | 36 |
| 4 | 2-18 | 0 | 41 | 1 | 11 | 3-15 | 0 | 21 | 1 | 3 | 1-13 | 0 | 15 | 1 | 14 | 6-12 | 0 | 30 | 1 |
| 6 | 2-18 | 0 | 15 | 1 | 13 | 3-15 | 0 | 46 | 1 | 5 | 1-13 | 58 | 61 | 35 | 16 | 6-12 | 0 | 12 | 1 |
| 8 | 2-18 | 30 | 18 | 29 | 1 | 5-15 | 69 | 94 | 68 | 7 | 1-13 | 0 | 41 | 1 | 0 | 8-12 | 88 | 99 | 87 |
| 2 | 4-18 | 20 | 20 | 20 | 3 | 5-15 | 55 | 57 | 55 | 9 | 1-13 | 0 | 28 | 1 | 2 | 8-12 | 48 | 68 | 48 |
| 4 | 4-18 | 35 | 11 | 35 | 5 | 5-15 | 0 | 40 | 1 | 11 | 1-13 | 29 | 30 | 29 | 4 | 8-12 | 35 | 25 | 34 |
| 6 | 4-18 | 0 | 20 | 1 | 7 | 5-15 | 41 | 30 | 40 | 13 | 1-13 | 33 | 30 | 33 | 6 | 8-12 | 0 | 86 | 1 |
| 0 | 6-18 | 49 | 10 | 48 | 9 | 5-15 | 46 | 4 | 45 | 15 | 1-13 | 0 | 14 | 1 | 8 | 8-12 | 56 | 45 | 55 |
| 2 | 6-18 | 0 | 32 | 1 | 11 | 5-15 | 0 | 31 | 1 | 1 | 3-13 | 135 | 138 | 10 | 10 | 8-12 | 82 | 57 | 25 |
| 4 | 6-18 | 53 | 14 | 52 | 13 | 5-15 | 0 | 18 | 1 | 3 | 3-13 | 0 | 37 | 1 | 12 | 8-12 | 55 | 44 | 54 |
| 6 | 6-18 | 0 | 10 | 1 | 1 | 7-15 | 0 | 54 | 1 | 5 | 3-13 | 77 | 51 | 20 | 14 | 8-12 | 0 | 18 | 1 |
| 2 | 8-18 | 27 | 11 | 27 | 3 | 7-15 | 0 | 26 | 1 | 7 | 3-13 | 27 | 25 | 26 | 16 | 8-12 | 17 | 13 | 17 |
| 4 | 8-18 | 62 | 26 | 62 | 5 | 7-15 | 0 | 26 | 1 | 9 | 3-13 | 45 | 45 | 44 | 2 | 10-12 | 48 | 57 | 47 |
| 1 | 1-17 | 0 | 31 | 1 | 7 | 7-15 | 0 | 48 | 1 | 11 | 3-13 | 0 | 14 | 1 | 4 | 10-12 | 141 | 132 | 11 |
| 3 | 1-17 | 63 | 58 | 63 | 9 | 7-15 | 0 | 61 | 1 | 13 | 3-13 | 0 | 41 | 1 | 6 | 10-12 | 0 | 28 | 1 |
| 5 | 1-17 | 0 | 49 | 1 | 11 | 7-15 | 0 | 14 | 1 | 15 | 3-13 | 54 | 45 | 53 | 8 | 10-12 | 0 | 66 | 1 |
| 7 | 1-17 | 44 | 16 | 43 | 13 | 7-15 | 0 | 11 | 1 | 1 | 5-13 | 54 | 51 | 53 | 10 | 10-12 | 28 | 23 | 28 |
| 9 | 1-17 | 0 | 22 | 1 | 1 | 9-15 | 40 | 27 | 40 | 3 | 5-13 | 80 | 88 | 69 | 12 | 10-12 | 0 | 24 | 1 |
| 1 | 3-17 | 0 | 20 | 1 | 3 | 9-15 | 0 | 27 | 1 | 5 | 5-13 | 47 | 39 | 47 | 14 | 10-12 | 68 | 13 | 45 |
| 3 | 3-17 | 70 | 35 | 70 | 5 | 9-15 | 0 | 28 | 1 | 7 | 5-13 | 54 | 61 | 54 | 0 | 12-12 | 84 | 77 | 56 |
| 5 | 3-17 | 0 | 42 | 1 | 7 | 9-15 | 53 | 48 | 52 | 9 | 5-13 | 51 | 46 | 50 | 4 | 12-12 | 0 | 14 | 1 |
| 7 | 3-17 | 39 | 7 | 38 | 9 | 9-15 | 0 | 40 | 1 | 11 | 5-13 | 29 | 18 | 28 | 6 | 12-12 | 0 | 41 | 1 |
| 9 | 3-17 | 0 | 14 | 1 | 11 | 9-15 | 0 | 9 | 1 | 13 | 5-13 | 66 | 39 | 66 | 8 | 12-12 | 0 | 62 | 1 |
| 1 | 5-17 | 45 | 56 | 45 | 1 | 11-15 | 0 | 14 | 1 | 15 | 5-13 | 0 | 10 | 1 | 10 | 12-12 | 0 | 10 | 1 |
| 3 | 5-17 | 0 | 5 | 1 | 3 | 11-15 | 0 | 5 | 1 | 1 | 7-13 | 91 | 111 | 26 | 12 | 12-12 | 0 | 28 | 1 |
| 5 | 5-17 | 45 | 25 | 45 | 5 | 11-15 | 0 | 19 | 1 | 3 | 7-13 | 63 | 42 | 42 | 12 | 12-12 | 0 | 28 | 1 |
| 7 | 5-17 | 0 | 10 | 1 | 7 | 11-15 | 51 | 37 | 51 | 5 | 7-13 | 66 | 74 | 65 | 14 | 12-12 | 0 | 25 | 1 |
| 9 | 5-17 | 0 | 14 | 1 | 9 | 11-15 | 57 | 26 | 56 | 7 | 7-13 | 40 | 35 | 39 | 2 | 14-12 | 79 | 30 | 65 |
| 1 | 7-17 | 0 | 4 | 1 | 1 | 13-15 | 0 | 14 | 1 | 9 | 7-13 | 0 | 42 | 1 | 4 | 14-12 | 69 | 80 | 68 |
| 3 | 7-17 | 47 | 11 | 47 | 3 | 13-15 | 47 | 11 | 47 | 11 | 7-13 | 42 | 39 | 42 | 6 | 14-12 | 62 | 67 | 62 |
| 5 | 7-17 | 0 | 18 | 1 | 5 | 13-15 | 32 | 20 | 32 | 13 | 7-13 | 66 | 14 | 53 | 8 | 14-12 | 0 | 31 | 1 |
| 7 | 7-17 | 61 | 43 | 61 | 7 | 13-15 | 50 | 21 | 50 | 15 | 7-13 | 0 | 18 | 1 | 10 | 14-12 | 0 | 15 | 1 |
| 9 | 7-17 | 74 | 45 | 73 | 1 | 15-15 | 0 | 18 | 1 | 1 | 9-13 | 0 | 31 | 1 | 12 | 14-12 | 40 | 17 | 40 |
| 1 | 9-17 | 0 | 31 | 1 | 3 | 15-15 | 0 | 9 | 1 | 3 | 9-13 | 72 | 103 | 56 | 0 | 16-12 | 43 | 17 | 43 |
| 3 | 9-17 | 0 | 9 | 1 | 2 | 0-14 | 58 | 58 | 58 | 5 | 9-13 | 63 | 60 | 62 | 2 | 16-12 | 76 | 12 | 76 |
| 5 | 9-17 | 0 | 31 | 1 | 6 | 0-14 | 0 | 73 | 1 | 7 | 9-13 | 0 | 42 | 1 | 4 | 16-12 | 0 | 23 | 1 |
| 7 | 9-17 | 0 | 18 | 1 | 10 | 0-14 | 0 | 23 | 1 | 9 | 9-13 | 59 | 47 | 59 | 6 | 16-12 | 62 | 74 | 62 |
| 1 | 11-17 | 0 | 25 | 1 | 14 | 0-14 | 0 | 37 | 1 | 11 | 9-13 | 28 | 43 | 27 | 8 | 16-12 | 0 | 25 | 1 |
| 3 | 11-17 | 0 | 7 | 1 | 0 | 2-14 | 58 | 54 | 57 | 13 | 9-13 | 60 | 23 | 59 | 10 | 16-12 | 0 | 26 | 1 |
| 0 | 0-16 | 0 | 8 | 1 | 2 | 2-14 | 0 | 62 | 1 | 1 | 11-13 | 33 | 41 | 33 | 2 | 18-12 | 0 | 38 | 1 |
| 4 | 0-16 | 0 | 78 | 1 | 4 | 2-14 | 49 | 39 | 48 | 3 | 11-13 | 70 | 100 | 38 | 4 | 18-12 | 0 | 15 | 1 |
| 8 | 0-16 | 0 | 17 | 1 | 6 | 2-14 | 0 | 17 | 1 | 5 | 11-13 | 0 | 53 | 1 | 6 | 18-12 | 32 | 41 | 31 |
| 12 | 0-16 | 116 | 79 | 32 | 8 | 2-14 | 0 | 33 | 1 | 7 | 11-13 | 0 | 52 | 1 | 1 | 1-11 | 349 | 353 | 4 |
| 2 | 2-16 | 0 | 50 | 1 | 10 | 2-14 | 0 | 5 | 1 | 9 | 11-13 | 38 | 26 | 37 | 3 | 1-11 | 142 | 154 | 8 |
| 4 | 2-16 | 0 | 8 | 1 | 12 | 2-14 | 55 | 18 | 55 | 11 | 11-13 | 0 | 25 | 1 | 5 | 1-11 | 66 | 85 | 31 |
| 6 | 2-16 | 0 | 15 | 1 | 14 | 2-14 | 0 | 40 | 1 | 13 | 11-13 | 28 | 14 | 28 | 7 | 1-11 | 154 | 149 | 10 |
| 8 | 2-16 | 0 | 11 | 1 | 2 | 4-14 | 60 | 72 | 51 | 1 | 13-13 | 0 | 12 | 1 | 9 | 1-11 | 155 | 158 | 17 |
| 10 | 2-16 | 40 | 34 | 39 | 4 | 4-14 | 54 | 35 | 54 | 3 | 13-13 | 9 | 16 | 9 | 11 | 1-11 | 0 | 34 | 1 |
| 12 | 2-16 | 0 | 28 | 1 | 6 | 4-14 | 0 | 25 | 1 | 5 | 13-13 | 0 | 35 | 1 | 13 | 1-11 | 0 | 29 | 1 |
| 0 | 4-16 | 65 | 57 | 65 | 8 | 4-14 | 34 | 39 | 33 | 7 | 13-13 | 71 | 19 | 70 | 15 | 1-11 | 0 | 44 | 1 |
| 2 | 4-16 | 0 | 50 | 1 | 10 | 4-14 | 0 | 15 | 1 | 9 | 13-13 | 0 | 10 | 1 | 17 | 1-11 | 0 | 28 | 1 |
| 4 | 4-16 | 42 | 52 | 42 | 12 | 4-14 | 0 | 24 | 1 | 11 | 13-13 | 73 | 23 | 73 | 1 | 3-11 | 428 | 429 | 4 |
| 6 | 4-16 | 0 | 29 | 1 | 14 | 4-14 | 0 | 21 | 1 | 1 | 15-13 | 41 | 10 | 41 | 3 | 3-11 | 135 | 144 | 15 |
| 8 | 4-16 | 72 | 2 | 40 | 0 | 6-14 | 0 | 156 | 1 | 3 | 15-13 | 0 | 27 | 1 | 5 | 3-11 | 104 | 114 | 22 |
| 10 | 4-16 | 68 | 33 | 68 | 2 | 6-14 | 65 | 39 | 41 | 5 | 15-13 | 39 | 29 | 38 | 7 | 3-11 | 102 | 75 | 30 |
| 12 | 4-16 | 0 | 35 | 1 | 4 | 6-14 | 0 | 24 | 1 | 7 | 15-13 | 0 | 49 | 1 | 9 | 3-11 | 73 | 78 | 29 |
| 2 | 6-16 | 57 | 55 | 57 | 6 | 6-14 | 59 | 40 | 43 | 9 | 15-13 | 87 | 43 | 87 | 11 | 3-11 | 0 | 91 | 1 |
| 4 | 6-16 | 0 | 14 | 1 | 8 | 6-14 | 0 | 15 | 1 | 1 | 17-13 | 38 | 29 | 37 | 13 | 3-11 | 42 | 16 | 41 |
| 6 | 6-16 | 0 | 27 | 1 | 10 | 6-14 | 0 | 42 | 1 | 3 | 17-13 | 70 | 6 | 70 | 15 | 3-11 | 0 | 51 | 1 |
| 8 | 6-16 | 47 | 49 | 46 | 12 | 6-14 | 0 | 7 | 1 | 5 | 17-13 | 73 | 28 | 73 | 17 | 3-11 | 52 | 41 | 51 |
| 10 | 6-16 | 0 | 21 | 1 | 14 | 6-14 | 0 | 11 | 1 | 0 | 0-12 | 524 | 549 | 9 | 1 | 5-11 | 340 | 342 | 6 |
| 0 | 8-16 | 0 | 36 | 1 | 2 | 8-14 | 75 | 50 | 27 | 4 | 0-12 | 196 | 186 | 10 | 3 | 5-11 | 224 | 215 | 8 |
| 2 | 8-16 | 0 | 37 | 1 | 4 | 8-14 | 66 | 46 | 34 | 8 | 0-12 | 111 | 139 | 70 | 5 | 5-11 | 0 | 56 | 1 |
| 4 | 8-16 | 0 | 9 | 1 | 6 | 8-14 | 69 | 50 | 68 | 12 | 0-12 | 76 | 85 | 75 | 7 | 5-11 | 154 | 160 | 9 |
| 6 | 8-16 | 0 | 62 | 1 | 8 | 8-14 | 66 | 81 | 65 | 16 | 0-12 | 46 | 67 | 46 | 9 | 5-11 | 0 | 14 | 1 |
| 8 | 8-16 | 0 | 12 | 1 | 10 | 8-14 | 0 | 8 | 1 | 2 | 2-12 | 149 | 147 | 8 | 11 | 5-11 | 0 | 53 | 1 |
| 10 | 8-16 | 59 | 36 | 59 | 12 | 8-14 | 0 | 14 | 1 | 4 | 2-12 | 70 | 93 | 70 | 13 | 5-11 | 0 | 37 | 1 |
| 2 | 10-16 | 41 | 25 | 40 | 14 | 8-14 | 0 | 11 | 1 | 6 | 2-12 | 129 | 146 | 10 | 15 | 5-11 | 0 | 45 | 1 |
| 4 | 10-16 | 37 | 24 | 37 | 0 | 10-14 | 60 | 43 | 60 | 8 | 2-12 | 0 | 74 | 1 | 17 | 5-11 | 37 | 15 | 37 |
| 6 | 10-16 | 45 | 3 | 45 | 2 | 10-14 | 0 | 26 | 1 | 10 | 2-12 | 0 | 18 | 1 | 1 | 7-11 | 210 | 210 | 7 |
| 8 | 10-16 | 67 | 57 | 67 | 4 | 10-14 | 0 | 44 | 1 | 12 | 2-12 | 0 | 45 | 1 | 3 | 7-11 | 224 | 227 | 7 |
| 0 | 12-16 | 60 | 43 | 60 | 6 | 10-14 | 0 | 30 | 1 | 14 | 2-12 | 45 | 52 | 44 | 5 | 7-11 | 54 | 88 | 53 |
| 2 | 12-16 | 0 | 13 | 1 | 8 | 10-14 | 19 | 14 | 17 | 16 | 2-12 | 0 | 34 | 1 | 7 | 7-11 | 162 | 146 | 9 |
| 4 | 12-16 | 53 | 14 | 52 | 10 | 10-14 | 0 | 12 | | | | | | | | | | | |

Table 10.

Observed and calculated structure factors for pchcl7a

Page 2

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|----|----|-----|------|------|-----|----|----|----|------|------|-----|----|----|----|------|------|-----|----|----|----|------|------|-----|----|----|----|------|------|-----|
| 16 | 10 | -10 | 0 | 6 | 1 | 13 | 11 | -9 | 47 | 49 | 46 | 0 | 12 | -8 | 84 | 92 | 37 | 15 | 9 | -7 | 0 | 76 | 1 | 4 | 8 | -6 | 178 | 195 | 7 |
| 2 | 12 | -10 | 67 | 83 | 67 | 15 | 11 | -9 | 63 | 24 | 63 | 2 | 12 | -8 | 201 | 170 | 10 | 17 | 9 | -7 | 0 | 38 | 1 | 6 | 8 | -6 | 298 | 298 | 7 |
| 4 | 12 | -10 | 199 | 204 | 11 | 17 | 11 | -9 | 71 | 23 | 70 | 4 | 12 | -8 | 100 | 82 | 100 | 19 | 9 | -7 | 21 | 17 | 20 | 8 | 8 | -6 | 379 | 374 | 6 |
| 6 | 12 | -10 | 84 | 59 | 30 | 1 | 13 | -9 | 50 | 54 | 49 | 6 | 12 | -8 | 45 | 21 | 45 | 1 | 11 | -7 | 336 | 316 | 7 | 10 | 8 | -6 | 290 | 289 | 10 |
| 8 | 12 | -10 | 0 | 29 | 1 | 3 | 13 | -9 | 122 | 119 | 17 | 8 | 12 | -8 | 78 | 45 | 43 | 3 | 11 | -7 | 299 | 298 | 7 | 12 | 8 | -6 | 47 | 57 | 47 |
| 10 | 12 | -10 | 0 | 20 | 1 | 5 | 13 | -9 | 85 | 81 | 28 | 10 | 12 | -8 | 61 | 29 | 60 | 5 | 11 | -7 | 58 | 67 | 57 | 14 | 8 | -6 | 0 | 56 | 1 |
| 12 | 12 | -10 | 98 | 34 | 51 | 7 | 13 | -9 | 52 | 43 | 51 | 12 | 12 | -8 | 33 | 14 | 32 | 7 | 11 | -7 | 100 | 108 | 24 | 16 | 8 | -6 | 115 | 115 | 33 |
| 14 | 12 | -10 | 0 | 19 | 1 | 9 | 13 | -9 | 37 | 10 | 36 | 14 | 12 | -8 | 0 | 33 | 1 | 9 | 11 | -7 | 142 | 161 | 14 | 18 | 8 | -6 | 0 | 22 | 1 |
| 16 | 12 | -10 | 77 | 24 | 76 | 11 | 13 | -9 | 0 | 33 | 1 | 16 | 12 | -8 | 0 | 8 | 1 | 11 | 11 | -7 | 77 | 67 | 32 | 20 | 8 | -6 | 0 | 13 | 1 |
| 0 | 14 | -10 | 0 | 30 | 1 | 13 | 13 | -9 | 0 | 19 | 1 | 2 | 14 | -8 | 90 | 98 | 72 | 13 | 11 | -7 | 0 | 33 | 1 | 0 | 10 | -6 | 230 | 205 | 10 |
| 2 | 14 | -10 | 91 | 53 | 91 | 15 | 13 | -9 | 50 | 19 | 50 | 4 | 14 | -8 | 64 | 21 | 48 | 15 | 11 | -7 | 0 | 46 | 1 | 2 | 10 | -6 | 0 | 12 | 1 |
| 4 | 14 | -10 | 75 | 62 | 62 | 1 | 15 | -9 | 70 | 49 | 69 | 6 | 14 | -8 | 83 | 49 | 83 | 17 | 11 | -7 | 73 | 61 | 72 | 4 | 10 | -6 | 99 | 134 | 48 |
| 6 | 14 | -10 | 0 | 64 | 1 | 3 | 15 | -9 | 0 | 46 | 1 | 8 | 14 | -8 | 0 | 55 | 1 | 1 | 13 | -7 | 125 | 124 | 16 | 6 | 10 | -6 | 121 | 108 | 13 |
| 8 | 14 | -10 | 0 | 31 | 1 | 5 | 15 | -9 | 26 | 7 | 26 | 10 | 14 | -8 | 34 | 28 | 33 | 5 | 13 | -7 | 159 | 174 | 12 | 8 | 10 | -6 | 142 | 142 | 12 |
| 10 | 14 | -10 | 0 | 14 | 1 | 7 | 15 | -9 | 0 | 69 | 1 | 12 | 14 | -8 | 38 | 24 | 38 | 3 | 13 | -7 | 164 | 179 | 13 | 10 | 10 | -6 | 137 | 144 | 15 |
| 12 | 14 | -10 | 0 | 32 | 1 | 9 | 15 | -9 | 0 | 9 | 1 | 14 | 14 | -8 | 22 | 20 | 22 | 7 | 13 | -7 | 156 | 145 | 16 | 12 | 10 | -6 | 68 | 29 | 38 |
| 14 | 14 | -10 | 65 | 24 | 65 | 11 | 15 | -9 | 58 | 29 | 58 | 16 | 14 | -8 | 0 | 8 | 1 | 9 | 13 | -7 | 50 | 80 | 50 | 10 | 10 | -6 | 0 | 39 | 1 |
| 2 | 16 | -10 | 0 | 53 | 1 | 13 | 15 | -9 | 0 | 18 | 1 | 0 | 16 | -8 | 69 | 77 | 68 | 11 | 13 | -7 | 65 | 73 | 65 | 16 | 10 | -6 | 0 | 18 | 1 |
| 4 | 16 | -10 | 41 | 66 | 41 | 1 | 17 | -9 | 0 | 31 | 1 | 2 | 16 | -8 | 0 | 22 | 1 | 13 | 13 | -7 | 0 | 18 | 1 | 18 | 10 | -6 | 0 | 57 | 1 |
| 6 | 16 | -10 | 0 | 69 | 1 | 3 | 17 | -9 | 41 | 48 | 40 | 4 | 16 | -8 | 0 | 22 | 1 | 15 | 13 | -7 | 0 | 27 | 1 | 2 | 12 | -6 | 90 | 59 | 19 |
| 8 | 16 | -10 | 69 | 56 | 68 | 5 | 17 | -9 | 0 | 32 | 1 | 6 | 16 | -8 | 60 | 61 | 60 | 17 | 13 | -7 | 63 | 33 | 63 | 4 | 12 | -6 | 106 | 132 | 16 |
| 10 | 16 | -10 | 0 | 16 | 1 | 7 | 17 | -9 | 43 | 34 | 42 | 8 | 16 | -8 | 0 | 39 | 1 | 1 | 15 | -7 | 101 | 90 | 36 | 6 | 12 | -6 | 92 | 98 | 35 |
| 12 | 16 | -10 | 43 | 20 | 43 | 9 | 17 | -9 | 50 | 26 | 49 | 10 | 16 | -8 | 0 | 11 | 1 | 3 | 15 | -7 | 51 | 50 | 50 | 8 | 12 | -6 | 226 | 212 | 10 |
| 0 | 18 | -10 | 0 | 60 | 1 | 11 | 17 | -9 | 92 | 21 | 43 | 12 | 16 | -8 | 0 | 33 | 1 | 5 | 15 | -7 | 40 | 63 | 40 | 10 | 12 | -6 | 0 | 38 | 1 |
| 2 | 18 | -10 | 0 | 35 | 1 | 1 | 19 | -9 | 0 | 49 | 1 | 14 | 16 | -8 | 0 | 29 | 1 | 7 | 15 | -7 | 0 | 67 | 1 | 12 | 12 | -6 | 0 | 50 | 1 |
| 4 | 18 | -10 | 67 | 31 | 66 | 3 | 19 | -9 | 52 | 36 | 51 | 2 | 18 | -8 | 62 | 61 | 62 | 9 | 15 | -7 | 26 | 30 | 25 | 14 | 12 | -6 | 51 | 20 | 51 |
| 6 | 18 | -10 | 0 | 54 | 1 | 5 | 19 | -9 | 21 | 21 | 21 | 4 | 18 | -8 | 0 | 60 | 1 | 11 | 15 | -7 | 0 | 31 | 1 | 16 | 12 | -6 | 135 | 115 | 39 |
| 8 | 18 | -10 | 0 | 37 | 1 | 7 | 19 | -9 | 54 | 13 | 53 | 6 | 18 | -8 | 0 | 38 | 1 | 13 | 15 | -7 | 0 | 27 | 1 | 18 | 12 | -6 | 0 | 20 | 1 |
| 10 | 18 | -10 | 0 | 34 | 1 | 9 | 19 | -9 | 96 | 42 | 40 | 8 | 18 | -8 | 0 | 5 | 1 | 15 | 15 | -7 | 40 | 19 | 39 | 0 | 14 | -6 | 306 | 323 | 11 |
| 2 | 20 | -10 | 0 | 50 | 1 | 1 | 21 | -9 | 49 | 26 | 49 | 10 | 18 | -8 | 44 | 35 | 44 | 1 | 17 | -7 | 0 | 15 | 1 | 2 | 14 | -6 | 194 | 208 | 10 |
| 4 | 20 | -10 | 59 | 20 | 58 | 3 | 21 | -9 | 0 | 17 | 1 | 12 | 18 | -8 | 0 | 25 | 1 | 3 | 17 | -7 | 119 | 115 | 23 | 4 | 14 | -6 | 104 | 88 | 19 |
| 6 | 20 | -10 | 72 | 18 | 71 | 5 | 21 | -9 | 65 | 12 | 64 | 0 | 20 | -8 | 42 | 34 | 41 | 5 | 17 | -7 | 117 | 86 | 117 | 6 | 14 | -6 | 148 | 141 | 15 |
| 1 | 1 | -9 | 394 | 334 | 3 | 0 | 0 | -8 | 343 | 317 | 7 | 2 | 20 | -8 | 30 | 15 | 30 | 7 | 17 | -7 | 81 | 65 | 77 | 8 | 14 | -6 | 0 | 31 | 1 |
| 3 | 1 | -9 | 62 | 62 | 20 | 4 | 0 | -8 | 336 | 345 | 7 | 4 | 20 | -8 | 41 | 41 | 40 | 9 | 17 | -7 | 0 | 45 | 1 | 10 | 14 | -6 | 30 | 41 | 29 |
| 5 | 1 | -9 | 214 | 222 | 4 | 8 | 0 | -8 | 115 | 84 | 25 | 6 | 20 | -8 | 18 | 24 | 17 | 11 | 17 | -7 | 0 | 34 | 1 | 12 | 14 | -6 | 0 | 34 | 1 |
| 7 | 1 | -9 | 127 | 114 | 13 | 12 | 0 | -8 | 117 | 101 | 51 | 8 | 20 | -8 | 0 | 21 | 1 | 13 | 17 | -7 | 19 | 28 | 18 | 14 | 14 | -6 | 56 | 19 | 55 |
| 9 | 1 | -9 | 132 | 114 | 13 | 16 | 0 | -8 | 0 | 15 | 1 | 2 | 22 | -8 | 73 | 19 | 72 | 1 | 19 | -7 | 0 | 21 | 1 | 16 | 14 | -6 | 0 | 13 | 1 |
| 11 | 1 | -9 | 117 | 124 | 11 | 20 | 0 | -8 | 0 | 20 | 1 | 4 | 22 | -8 | 26 | 38 | 25 | 3 | 19 | -7 | 0 | 50 | 1 | 2 | 16 | -6 | 69 | 87 | 68 |
| 13 | 1 | -9 | 35 | 33 | 34 | 2 | 2 | -8 | 123 | 114 | 6 | 1 | 1 | -7 | 294 | 291 | 3 | 5 | 19 | -7 | 92 | 100 | 79 | 4 | 16 | -6 | 0 | 96 | 1 |
| 15 | 1 | -9 | 0 | 25 | 1 | 4 | 2 | -8 | 134 | 137 | 6 | 3 | 1 | -7 | 541 | 478 | 7 | 7 | 19 | -7 | 43 | 18 | 43 | 6 | 16 | -6 | 130 | 126 | 17 |
| 17 | 1 | -9 | 37 | 18 | 36 | 6 | 2 | -8 | 89 | 99 | 13 | 5 | 1 | -7 | 264 | 260 | 4 | 9 | 19 | -7 | 0 | 16 | 1 | 8 | 16 | -6 | 46 | 59 | 46 |
| 19 | 1 | -9 | 0 | 8 | 1 | 8 | 2 | -8 | 144 | 153 | 11 | 7 | 1 | -7 | 224 | 202 | 6 | 11 | 19 | -7 | 0 | 44 | 1 | 10 | 16 | -6 | 122 | 94 | 25 |
| 1 | 3 | -9 | 180 | 183 | 5 | 10 | 2 | -8 | 214 | 217 | 8 | 9 | 1 | -7 | 226 | 220 | 4 | 1 | 21 | -7 | 0 | 27 | 1 | 12 | 16 | -6 | 0 | 31 | 1 |
| 3 | 3 | -9 | 96 | 101 | 8 | 12 | 2 | -8 | 34 | 57 | 34 | 11 | 1 | -7 | 309 | 312 | 5 | 3 | 21 | -7 | 86 | 71 | 49 | 14 | 16 | -6 | 0 | 27 | 1 |
| 5 | 3 | -9 | 98 | 80 | 10 | 14 | 2 | -8 | 54 | 52 | 53 | 13 | 1 | -7 | 186 | 190 | 7 | 5 | 21 | -7 | 46 | 38 | 46 | 0 | 18 | -6 | 62 | 34 | 61 |
| 7 | 3 | -9 | 121 | 121 | 9 | 16 | 2 | -8 | 34 | 26 | 34 | 15 | 1 | -7 | 23 | 23 | 22 | 7 | 21 | -7 | 0 | 8 | 1 | 2 | 18 | -6 | 87 | 107 | 50 |
| 9 | 3 | -9 | 207 | 196 | 9 | 18 | 2 | -8 | 0 | 13 | 1 | 17 | 1 | -7 | 0 | 22 | 1 | 9 | 21 | -7 | 52 | 5 | 52 | 4 | 18 | -6 | 0 | 47 | 1 |
| 11 | 3 | -9 | 64 | 61 | 35 | 20 | 2 | -8 | 42 | 14 | 41 | 19 | 1 | -7 | 33 | 32 | 33 | 1 | 23 | -7 | 0 | 19 | 1 | 6 | 18 | -6 | 75 | 83 | 74 |
| 13 | 3 | -9 | 62 | 54 | 61 | 0 | 4 | -8 | 412 | 339 | 5 | 21 | 1 | -7 | 0 | 21 | 1 | 3 | 23 | -7 | 0 | 19 | 1 | 8 | 18 | -6 | 0 | 18 | 1 |
| 15 | 3 | -9 | 0 | 39 | 1 | 2 | 4 | -8 | 169 | 121 | 6 | 1 | 3 | -7 | 420 | 415 | 4 | 2 | 0 | -6 | 513 | 522 | 7 | 10 | 18 | -6 | 0 | 28 | 1 |
| 17 | 3 | -9 | 58 | 18 | 57 | 4 | 4 | -8 | 235 | 204 | 7 | 3 | 3 | -7 | 570 | 560 | 8 | 6 | 0 | -6 | 185 | 186 | 9 | 12 | 18 | -6 | 0 | 43 | 1 |
| 19 | 3 | -9 | 0 | 12 | 1 | 6 | 4 | -8 | 308 | 318 | 7 | 5 | 3 | -7 | 271 | 225 | 7 | 10 | 0 | -6 | 201 | 210 | 8 | 14 | 18 | -6 | 34 | 12 | 33 |
| 1 | 5 | -9 | 257 | 262 | 4 | 8 | 4 | -8 | 122 | 132 | 22 | 7 | 3 | -7 | 116 | 122 | 11 | 14 | 0 | -6 | 138 | 134 | 15 | 2 | 20 | -6 | 79 | 25 | 78 |
| 3 | 5 | -9 | 167 | 186 | 6 | 10 | 4 | -8 | 60 | 56 | 50 | 9 | 3 | -7 | 143 | 152 | 10 | 18 | 0 | -6 | 0 | 26 | 1 | 4 | 20 | -6 | 107 | 106 | 107 |
| 5 | 5 | -9 | 114 | 144 | 27 | 12 | 4 | -8 | 0 | 21 | 1 | 11 | 3 | -7 | 110 | 85 | 11 | 0 | 2 | -6 | 367 | 310 | 4 | 6 | 20 | -6 | 68 | 73 | 67 |
| 7 | 5 | -9 | 97 | 108 | 22 | 14 | 4 | -8 | 86 | 100 | 32 | 13 | 3 | -7 | 122 | 118 | 16 | 2 | 2 | -6 | 524 | 514 | 4 | 8 | 20 | -6 | 0 | 22 | 1 |
| 9 | 5 | -9 | 92 | 101 | 16 | 16 | 4 | -8 | 41 | 29 | 41 | 15 | 3 | -7 | 0 | 24 | 1 | 4 | 2 | -6 | 922 | 940 | 8 | 10 | 20 | -6 | 50 | 51 | 49 |
| 11 | 5 | -9 | 64 | 70 | 25 | 18 | 4 | -8 | 53 | 18 | 53 | 17 | 3 | -7 | 0 | 19 | 1 | 6 | 2 | -6 | 170 | 181 | 6 | 0 | 22 | -6 | 0 | 24 | 1 |
| 13 | 5 | -9 | 0 | 40 | 1 | 20 | 4 | -8 | 44 | 22 | 43 | | | | | | | | | | | | | | | | | | |

Table 10. Observed and calculated structure factors for pchcl7a

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|----|----|----|------|------|-----|----|----|----|------|------|-----|----|----|----|------|------|-----|----|----|----|------|------|-----|----|----|----|------|------|-----|
| 7 | 5 | -5 | 343 | 366 | 4 | 6 | 2 | -4 | 541 | 562 | 8 | 2 | 20 | -4 | 0 | 31 | 1 | 1 | 15 | -3 | 178 | 172 | 11 | 6 | 10 | -2 | 311 | 293 | 6 |
| 9 | 5 | -5 | 289 | 295 | 6 | 8 | 2 | -4 | 241 | 261 | 3 | 4 | 20 | -4 | 0 | 34 | 1 | 3 | 15 | -3 | 84 | 68 | 32 | 8 | 10 | -2 | 178 | 169 | 9 |
| 11 | 5 | -5 | 253 | 257 | 6 | 10 | 2 | -4 | 142 | 138 | 16 | 6 | 20 | -4 | 78 | 51 | 78 | 5 | 15 | -3 | 96 | 121 | 39 | 10 | 10 | -2 | 88 | 84 | 20 |
| 13 | 5 | -5 | 222 | 216 | 7 | 12 | 2 | -4 | 187 | 180 | 9 | 8 | 20 | -4 | 0 | 28 | 1 | 7 | 15 | -3 | 0 | 122 | 1 | 12 | 10 | -2 | 0 | 94 | 1 |
| 15 | 5 | -5 | 116 | 133 | 39 | 14 | 2 | -4 | 154 | 141 | 8 | 10 | 20 | -4 | 0 | 13 | 1 | 9 | 15 | -3 | 41 | 29 | 40 | 14 | 10 | -2 | 0 | 88 | 1 |
| 17 | 5 | -5 | 56 | 62 | 56 | 16 | 2 | -4 | 90 | 92 | 19 | 12 | 20 | -4 | 0 | 34 | 1 | 11 | 15 | -3 | 64 | 44 | 63 | 16 | 10 | -2 | 0 | 16 | 1 |
| 19 | 5 | -5 | 0 | 18 | 1 | 18 | 2 | -4 | 0 | 21 | 1 | 4 | 22 | -4 | 0 | 35 | 1 | 13 | 15 | -3 | 26 | 15 | 26 | 18 | 10 | -2 | 90 | 14 | 36 |
| 21 | 5 | -5 | 46 | 19 | 46 | 20 | 2 | -4 | 43 | 11 | 42 | 2 | 22 | -4 | 0 | 77 | 1 | 15 | 15 | -3 | 0 | 19 | 1 | 20 | 10 | -2 | 31 | 11 | 30 |
| 1 | 7 | -5 | 571 | 559 | 8 | 22 | 2 | -4 | 0 | 18 | 1 | 6 | 22 | -4 | 0 | 19 | 1 | 17 | 15 | -3 | 51 | 13 | 51 | 2 | 12 | -2 | 216 | 219 | 6 |
| 3 | 7 | -5 | 197 | 218 | 6 | 0 | 4 | -4 | 869 | 886 | 7 | 8 | 22 | -4 | 0 | 29 | 1 | 1 | 17 | -3 | 0 | 69 | 1 | 4 | 12 | -2 | 325 | 297 | 6 |
| 5 | 7 | -5 | 143 | 138 | 8 | 2 | 4 | -4 | 631 | 657 | 7 | 0 | 24 | -4 | 0 | 50 | 1 | 3 | 17 | -3 | 0 | 27 | 1 | 6 | 12 | -2 | 167 | 157 | 34 |
| 7 | 7 | -5 | 204 | 225 | 16 | 4 | 4 | -4 | 226 | 252 | 6 | 2 | 24 | -4 | 43 | 25 | 43 | 5 | 17 | -3 | 76 | 65 | 76 | 8 | 12 | -2 | 194 | 193 | 16 |
| 9 | 7 | -5 | 293 | 283 | 8 | 6 | 4 | -4 | 723 | 777 | 6 | 4 | 24 | -4 | 0 | 27 | 1 | 7 | 17 | -3 | 0 | 35 | 1 | 10 | 12 | -2 | 66 | 17 | 65 |
| 11 | 7 | -5 | 283 | 272 | 7 | 8 | 4 | -4 | 185 | 193 | 8 | 1 | 1 | -3 | 1945 | 2039 | 14 | 9 | 17 | -3 | 45 | 53 | 45 | 12 | 12 | -2 | 13 | 35 | 12 |
| 13 | 7 | -5 | 104 | 104 | 25 | 10 | 4 | -4 | 475 | 470 | 4 | 3 | 1 | -3 | 1118 | 1181 | 13 | 11 | 17 | -3 | 0 | 42 | 1 | 14 | 12 | -2 | 0 | 9 | 1 |
| 15 | 7 | -5 | 148 | 146 | 39 | 12 | 4 | -4 | 204 | 202 | 7 | 5 | 1 | -3 | 364 | 334 | 4 | 13 | 17 | -3 | 0 | 37 | 1 | 16 | 12 | -2 | 0 | 26 | 1 |
| 17 | 7 | -5 | 0 | 52 | 1 | 14 | 4 | -4 | 197 | 199 | 8 | 7 | 1 | -3 | 380 | 371 | 2 | 15 | 17 | -3 | 0 | 25 | 1 | 18 | 12 | -2 | 0 | 13 | 1 |
| 19 | 7 | -5 | 0 | 37 | 1 | 16 | 4 | -4 | 0 | 55 | 1 | 9 | 1 | -3 | 182 | 182 | 4 | 1 | 19 | -3 | 24 | 31 | 23 | 0 | 14 | -2 | 266 | 246 | 11 |
| 1 | 9 | -5 | 409 | 437 | 4 | 18 | 4 | -4 | 61 | 15 | 61 | 11 | 1 | -3 | 93 | 81 | 12 | 3 | 19 | -3 | 0 | 33 | 1 | 2 | 14 | -2 | 165 | 160 | 15 |
| 3 | 9 | -5 | 161 | 151 | 42 | 20 | 4 | -4 | 45 | 51 | 45 | 13 | 1 | -3 | 102 | 86 | 49 | 5 | 19 | -3 | 92 | 76 | 34 | 4 | 14 | -2 | 139 | 138 | 13 |
| 5 | 9 | -5 | 0 | 43 | 1 | 2 | 6 | -4 | 394 | 407 | 6 | 15 | 1 | -3 | 66 | 58 | 24 | 7 | 19 | -3 | 0 | 26 | 1 | 6 | 14 | -2 | 135 | 140 | 14 |
| 7 | 9 | -5 | 210 | 207 | 10 | 4 | 6 | -4 | 89 | 72 | 10 | 17 | 1 | -3 | 32 | 36 | 31 | 9 | 19 | -3 | 45 | 28 | 44 | 8 | 14 | -2 | 0 | 56 | 1 |
| 9 | 9 | -5 | 188 | 197 | 25 | 6 | 6 | -4 | 300 | 336 | 7 | 19 | 1 | -3 | 41 | 34 | 41 | 11 | 19 | -3 | 21 | 22 | 20 | 10 | 14 | -2 | 63 | 65 | 62 |
| 11 | 9 | -5 | 78 | 60 | 37 | 8 | 6 | -4 | 166 | 152 | 7 | 21 | 1 | -3 | 0 | 26 | 1 | 13 | 19 | -3 | 0 | 16 | 1 | 12 | 14 | -2 | 74 | 48 | 74 |
| 13 | 9 | -5 | 47 | 35 | 47 | 10 | 6 | -4 | 414 | 426 | 5 | 1 | 3 | -3 | 789 | 771 | 6 | 1 | 21 | -3 | 62 | 9 | 61 | 14 | 14 | -2 | 38 | 32 | 38 |
| 15 | 9 | -5 | 98 | 103 | 28 | 12 | 6 | -4 | 112 | 106 | 17 | 3 | 3 | -3 | 757 | 740 | 5 | 3 | 21 | -3 | 22 | 33 | 22 | 16 | 14 | -2 | 41 | 18 | 40 |
| 17 | 9 | -5 | 90 | 70 | 36 | 14 | 6 | -4 | 141 | 122 | 42 | 5 | 3 | -3 | 880 | 899 | 14 | 5 | 21 | -3 | 71 | 30 | 71 | 18 | 14 | -2 | 0 | 29 | 1 |
| 19 | 9 | -5 | 30 | 15 | 29 | 16 | 6 | -4 | 79 | 80 | 79 | 7 | 3 | -3 | 404 | 389 | 5 | 7 | 21 | -3 | 78 | 42 | 59 | 2 | 16 | -2 | 103 | 132 | 38 |
| 1 | 11 | -5 | 318 | 322 | 11 | 18 | 6 | -4 | 61 | 52 | 61 | 9 | 3 | -3 | 220 | 200 | 4 | 9 | 21 | -3 | 42 | 27 | 42 | 4 | 16 | -2 | 133 | 123 | 15 |
| 3 | 11 | -5 | 208 | 209 | 7 | 20 | 6 | -4 | 49 | 21 | 49 | 11 | 3 | -3 | 87 | 100 | 16 | 11 | 21 | -3 | 55 | 10 | 55 | 6 | 16 | -2 | 123 | 127 | 27 |
| 5 | 11 | -5 | 30 | 16 | 29 | 0 | 8 | -4 | 585 | 599 | 8 | 13 | 3 | -3 | 124 | 123 | 23 | 1 | 23 | -3 | 0 | 17 | 1 | 8 | 16 | -2 | 0 | 82 | 1 |
| 7 | 11 | -5 | 190 | 217 | 10 | 2 | 8 | -4 | 476 | 525 | 4 | 15 | 3 | -3 | 81 | 91 | 31 | 3 | 23 | -3 | 72 | 58 | 71 | 10 | 16 | -2 | 56 | 11 | 56 |
| 9 | 11 | -5 | 268 | 285 | 9 | 4 | 8 | -4 | 53 | 73 | 28 | 17 | 3 | -3 | 37 | 33 | 36 | 5 | 23 | -3 | 68 | 35 | 68 | 12 | 16 | -2 | 0 | 36 | 1 |
| 11 | 11 | -5 | 0 | 49 | 1 | 6 | 8 | -4 | 96 | 101 | 41 | 19 | 3 | -3 | 0 | 30 | 1 | 7 | 23 | -3 | 0 | 2 | 1 | 14 | 16 | -2 | 62 | 45 | 61 |
| 13 | 11 | -5 | 0 | 49 | 1 | 8 | 8 | -4 | 137 | 118 | 11 | 21 | 3 | -3 | 0 | 29 | 1 | 2 | 0 | -2 | 1775 | 1860 | 25 | 16 | 16 | -2 | 0 | 28 | 1 |
| 15 | 11 | -5 | 70 | 40 | 70 | 10 | 8 | -4 | 105 | 104 | 16 | 1 | 5 | -3 | 332 | 329 | 2 | 6 | 0 | -2 | 866 | 994 | 15 | 0 | 18 | -2 | 0 | 63 | 1 |
| 17 | 11 | -5 | 73 | 78 | 72 | 12 | 8 | -4 | 122 | 94 | 18 | 3 | 5 | -3 | 990 | 972 | 7 | 10 | 0 | -2 | 190 | 177 | 14 | 2 | 18 | -2 | 82 | 80 | 49 |
| 19 | 11 | -5 | 0 | 14 | 1 | 14 | 8 | -4 | 159 | 158 | 22 | 5 | 5 | -3 | 510 | 507 | 5 | 14 | 0 | -2 | 167 | 168 | 16 | 4 | 18 | -2 | 0 | 17 | 1 |
| 1 | 13 | -5 | 222 | 220 | 9 | 16 | 8 | -4 | 73 | 53 | 72 | 7 | 5 | -3 | 0 | 74 | 1 | 18 | 0 | -2 | 0 | 38 | 1 | 6 | 18 | -2 | 48 | 82 | 48 |
| 3 | 13 | -5 | 111 | 112 | 16 | 18 | 8 | -4 | 55 | 59 | 54 | 9 | 5 | -3 | 345 | 361 | 5 | 22 | 0 | -2 | 0 | 15 | 1 | 8 | 18 | -2 | 37 | 26 | 37 |
| 5 | 13 | -5 | 0 | 45 | 1 | 20 | 8 | -4 | 0 | 6 | 1 | 11 | 5 | -3 | 77 | 82 | 31 | 0 | 2 | -2 | 2282 | 2179 | 5 | 10 | 18 | -2 | 32 | 42 | 31 |
| 7 | 13 | -5 | 254 | 286 | 20 | 2 | 10 | -4 | 285 | 277 | 5 | 13 | 5 | -3 | 41 | 56 | 40 | 2 | 2 | -2 | 2555 | 2533 | 7 | 12 | 18 | -2 | 75 | 29 | 74 |
| 9 | 13 | -5 | 182 | 187 | 37 | 4 | 10 | -4 | 146 | 133 | 9 | 15 | 5 | -3 | 43 | 60 | 43 | 4 | 2 | -2 | 690 | 697 | 4 | 14 | 18 | -2 | 0 | 17 | 1 |
| 11 | 13 | -5 | 0 | 40 | 1 | 6 | 10 | -4 | 213 | 196 | 7 | 17 | 5 | -3 | 0 | 27 | 1 | 6 | 2 | -2 | 297 | 339 | 3 | 2 | 20 | -2 | 13 | 21 | 13 |
| 13 | 13 | -5 | 0 | 24 | 1 | 8 | 10 | -4 | 453 | 440 | 5 | 19 | 5 | -3 | 0 | 33 | 1 | 8 | 2 | -2 | 298 | 291 | 8 | 4 | 20 | -2 | 0 | 62 | 1 |
| 15 | 13 | -5 | 35 | 35 | 35 | 10 | 10 | -4 | 72 | 95 | 43 | 21 | 5 | -3 | 76 | 4 | 76 | 10 | 2 | -2 | 250 | 233 | 5 | 6 | 20 | -2 | 0 | 26 | 1 |
| 17 | 13 | -5 | 0 | 52 | 1 | 12 | 10 | -4 | 0 | 106 | 1 | 1 | 7 | -3 | 238 | 233 | 4 | 12 | 2 | -2 | 67 | 68 | 34 | 8 | 20 | -2 | 81 | 66 | 47 |
| 1 | 15 | -5 | 84 | 65 | 25 | 14 | 10 | -4 | 52 | 34 | 52 | 3 | 7 | -3 | 310 | 329 | 5 | 14 | 2 | -2 | 99 | 103 | 34 | 10 | 20 | -2 | 0 | 35 | 1 |
| 3 | 15 | -5 | 182 | 174 | 11 | 16 | 10 | -4 | 0 | 87 | 1 | 5 | 7 | -3 | 490 | 509 | 9 | 16 | 2 | -2 | 0 | 58 | 1 | 12 | 20 | -2 | 13 | 6 | 12 |
| 5 | 15 | -5 | 127 | 134 | 40 | 18 | 10 | -4 | 0 | 13 | 1 | 7 | 7 | -3 | 412 | 371 | 5 | 18 | 2 | -2 | 84 | 85 | 46 | 0 | 22 | -2 | 0 | 41 | 1 |
| 7 | 15 | -5 | 164 | 173 | 15 | 20 | 10 | -4 | 39 | 11 | 39 | 9 | 7 | -3 | 145 | 129 | 26 | 20 | 2 | -2 | 35 | 22 | 35 | 2 | 22 | -2 | 0 | 26 | 1 |
| 9 | 15 | -5 | 53 | 44 | 52 | 0 | 12 | -4 | 434 | 417 | 8 | 11 | 7 | -3 | 79 | 81 | 22 | 22 | 2 | -2 | 0 | 4 | 1 | 4 | 22 | -2 | 0 | 17 | 1 |
| 11 | 15 | -5 | 45 | 54 | 44 | 2 | 12 | -4 | 73 | 96 | 72 | 13 | 7 | -3 | 134 | 129 | 22 | 2 | 4 | -2 | 1209 | 1201 | 9 | 6 | 22 | -2 | 0 | 5 | 1 |
| 13 | 15 | -5 | 0 | 41 | 1 | 4 | 12 | -4 | 34 | 44 | 33 | 15 | 7 | -3 | 127 | 136 | 21 | 4 | 4 | -2 | 82 | 78 | 8 | 8 | 22 | -2 | 0 | 18 | 1 |
| 15 | 15 | -5 | 0 | 31 | 1 | 6 | 12 | -4 | 198 | 217 | 9 | 17 | 7 | -3 | 0 | 30 | 1 | 6 | 4 | -2 | 353 | 355 | 4 | 10 | 22 | -2 | 0 | 22 | 1 |
| 17 | 15 | -5 | 0 | 43 | 1 | 8 | 12 | -4 | 120 | 102 | 26 | 19 | 7 | -3 | 0 | 13 | 1 | 8 | 4 | -2 | 518 | 502 | 6 | 2 | 24 | -2 | 45 | 24 | 44 |
| 1 | 17 | -5 | 40 | 47 | 40 | 10 | 12 | -4 | 98 | 114 | 22 | 21 | 7 | -3 | 0 | 13 | 1 | 10 | 4 | -2 | 159 | 152 | 35 | 4 | 24 | -2 | 36 | 28 | 35 |
| 3 | 17 | -5 | 87 | 90 | 28 | 12 | 12 | -4 | 0 | 59 | 1 | 1 | 9 | -3 | 532 | 538 | 23 | 12 | 4 | -2 | 0 | 79 | 1 | 6 | 24 | -2 | 0 | 26 | 1 |
| 5 | 17 | -5 | 109 | 135 | 36 | 14 | 12 | -4 | 37 | 29 | 37 | 3 | | | | | | | | | | | | | | | | | |

Table 10. Observed and calculated structure factors for pchcl7a

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|----|----|----|------|------|-----|----|----|---|------|------|-----|----|----|---|------|------|-----|----|----|---|------|------|-----|----|----|---|------|------|-----|
| 15 | 5 | -1 | 0 | 67 | 1 | 6 | 2 | 0 | 229 | 168 | 13 | 14 | 18 | 0 | 28 | 11 | 28 | 11 | 13 | 1 | 115 | 105 | 24 | 6 | 10 | 2 | 308 | 293 | 5 |
| 17 | 5 | -1 | 0 | 22 | 1 | 8 | 2 | 0 | 511 | 457 | 10 | 0 | 20 | 0 | 91 | 126 | 90 | 13 | 13 | 1 | 76 | 57 | 40 | 8 | 10 | 2 | 177 | 169 | 9 |
| 19 | 5 | -1 | 0 | 13 | 1 | 10 | 2 | 0 | 161 | 158 | 7 | 2 | 20 | 0 | 37 | 23 | 37 | 15 | 13 | 1 | 0 | 29 | 1 | 10 | 10 | 2 | 92 | 84 | 75 |
| 21 | 5 | -1 | 48 | 29 | 47 | 12 | 2 | 0 | 80 | 83 | 80 | 4 | 20 | 0 | 59 | 24 | 58 | 17 | 13 | 1 | 0 | 25 | 1 | 12 | 10 | 2 | 0 | 94 | 1 |
| 1 | 7 | -1 | 853 | 871 | 6 | 14 | 2 | 0 | 189 | 182 | 11 | 6 | 20 | 0 | 98 | 82 | 43 | 19 | 13 | 1 | 53 | 15 | 53 | 14 | 10 | 2 | 87 | 88 | 87 |
| 3 | 7 | -1 | 1277 | 1321 | 8 | 16 | 2 | 0 | 101 | 105 | 21 | 8 | 20 | 0 | 0 | 82 | 1 | 1 | 15 | 1 | 101 | 117 | 18 | 16 | 10 | 2 | 0 | 16 | 1 |
| 5 | 7 | -1 | 538 | 515 | 5 | 18 | 2 | 0 | 0 | 18 | 1 | 10 | 20 | 0 | 41 | 34 | 41 | 3 | 15 | 1 | 296 | 291 | 7 | 18 | 10 | 2 | 47 | 14 | 46 |
| 7 | 7 | -1 | 97 | 92 | 11 | 20 | 2 | 0 | 57 | 17 | 57 | 12 | 20 | 0 | 67 | 32 | 66 | 5 | 15 | 1 | 229 | 226 | 10 | 20 | 10 | 2 | 60 | 11 | 60 |
| 9 | 7 | -1 | 153 | 163 | 9 | 22 | 2 | 0 | 0 | 34 | 1 | 2 | 22 | 0 | 48 | 46 | 47 | 7 | 15 | 1 | 185 | 173 | 27 | 2 | 12 | 2 | 215 | 219 | 6 |
| 11 | 7 | -1 | 303 | 317 | 7 | 0 | 4 | 0 | 2075 | 2224 | 6 | 4 | 22 | 0 | 48 | 7 | 48 | 9 | 15 | 1 | 80 | 97 | 80 | 4 | 12 | 2 | 329 | 297 | 6 |
| 13 | 7 | -1 | 101 | 83 | 18 | 2 | 4 | 0 | 3623 | 3581 | 5 | 6 | 22 | 0 | 46 | 25 | 46 | 11 | 15 | 1 | 0 | 70 | 1 | 6 | 12 | 2 | 166 | 157 | 31 |
| 15 | 7 | -1 | 102 | 124 | 102 | 4 | 4 | 0 | 1041 | 1269 | 10 | 8 | 22 | 0 | 114 | 101 | 32 | 13 | 15 | 1 | 37 | 19 | 36 | 8 | 12 | 2 | 196 | 193 | 12 |
| 17 | 7 | -1 | 0 | 57 | 1 | 6 | 4 | 0 | 420 | 448 | 11 | 10 | 22 | 0 | 51 | 20 | 51 | 15 | 15 | 1 | 64 | 40 | 64 | 10 | 12 | 2 | 64 | 17 | 63 |
| 19 | 7 | -1 | 49 | 50 | 48 | 8 | 4 | 0 | 365 | 355 | 4 | 0 | 24 | 0 | 140 | 85 | 37 | 17 | 15 | 1 | 0 | 5 | 1 | 12 | 12 | 2 | 56 | 35 | 56 |
| 21 | 7 | -1 | 0 | 41 | 1 | 10 | 4 | 0 | 400 | 401 | 5 | 2 | 24 | 0 | 45 | 16 | 45 | 1 | 17 | 1 | 200 | 201 | 16 | 14 | 12 | 2 | 62 | 9 | 62 |
| 1 | 9 | -1 | 139 | 146 | 10 | 12 | 4 | 0 | 0 | 64 | 1 | 4 | 24 | 0 | 0 | 17 | 1 | 3 | 17 | 1 | 0 | 30 | 1 | 16 | 12 | 2 | 0 | 26 | 1 |
| 3 | 9 | -1 | 929 | 923 | 9 | 14 | 4 | 0 | 216 | 199 | 14 | 6 | 24 | 0 | 51 | 13 | 51 | 5 | 17 | 1 | 72 | 46 | 72 | 18 | 12 | 2 | 22 | 13 | 21 |
| 5 | 9 | -1 | 132 | 129 | 9 | 16 | 4 | 0 | 89 | 110 | 47 | 1 | 1 | 1 | 1202 | 1177 | 3 | 7 | 17 | 1 | 135 | 138 | 17 | 0 | 14 | 2 | 274 | 246 | 11 |
| 7 | 9 | -1 | 325 | 326 | 5 | 18 | 4 | 0 | 38 | 35 | 38 | 3 | 1 | 1 | 1800 | 1811 | 6 | 9 | 17 | 1 | 0 | 23 | 1 | 2 | 14 | 2 | 173 | 160 | 12 |
| 9 | 9 | -1 | 187 | 179 | 8 | 20 | 4 | 0 | 0 | 25 | 1 | 5 | 1 | 1 | 905 | 898 | 9 | 11 | 17 | 1 | 47 | 26 | 46 | 4 | 14 | 2 | 147 | 138 | 16 |
| 11 | 9 | -1 | 70 | 62 | 69 | 22 | 4 | 0 | 0 | 27 | 1 | 7 | 1 | 1 | 628 | 624 | 8 | 13 | 17 | 1 | 59 | 58 | 59 | 6 | 14 | 2 | 138 | 140 | 14 |
| 13 | 9 | -1 | 241 | 230 | 9 | 2 | 6 | 0 | 1253 | 1267 | 19 | 9 | 1 | 1 | 281 | 300 | 7 | 15 | 17 | 1 | 70 | 13 | 69 | 8 | 14 | 2 | 74 | 56 | 36 |
| 15 | 9 | -1 | 45 | 56 | 45 | 4 | 6 | 0 | 72 | 86 | 11 | 11 | 1 | 1 | 74 | 59 | 25 | 1 | 19 | 1 | 66 | 52 | 65 | 10 | 14 | 2 | 0 | 65 | 1 |
| 17 | 9 | -1 | 0 | 14 | 1 | 6 | 6 | 0 | 1280 | 1294 | 8 | 13 | 1 | 1 | 139 | 122 | 18 | 3 | 19 | 1 | 0 | 45 | 1 | 12 | 14 | 2 | 0 | 48 | 1 |
| 19 | 9 | -1 | 69 | 32 | 69 | 8 | 6 | 0 | 168 | 154 | 6 | 15 | 1 | 1 | 105 | 122 | 104 | 5 | 19 | 1 | 59 | 65 | 59 | 14 | 14 | 2 | 36 | 32 | 35 |
| 21 | 9 | -1 | 63 | 28 | 62 | 10 | 6 | 0 | 74 | 82 | 18 | 17 | 1 | 1 | 0 | 44 | 1 | 7 | 19 | 1 | 83 | 94 | 77 | 16 | 14 | 2 | 0 | 18 | 1 |
| 1 | 11 | -1 | 230 | 233 | 6 | 12 | 6 | 0 | 0 | 78 | 1 | 19 | 1 | 1 | 0 | 21 | 1 | 9 | 19 | 1 | 0 | 79 | 1 | 18 | 14 | 2 | 0 | 29 | 1 |
| 3 | 11 | -1 | 440 | 442 | 11 | 14 | 6 | 0 | 89 | 133 | 88 | 21 | 1 | 1 | 0 | 21 | 1 | 11 | 19 | 1 | 0 | 20 | 1 | 2 | 16 | 2 | 113 | 132 | 32 |
| 5 | 11 | -1 | 275 | 268 | 7 | 16 | 6 | 0 | 0 | 48 | 1 | 1 | 3 | 1 | 2125 | 2055 | 4 | 13 | 19 | 1 | 0 | 22 | 1 | 4 | 16 | 2 | 137 | 123 | 14 |
| 7 | 11 | -1 | 88 | 74 | 20 | 20 | 6 | 0 | 51 | 42 | 50 | 5 | 3 | 1 | 453 | 439 | 3 | 1 | 21 | 1 | 0 | 64 | 1 | 6 | 16 | 2 | 116 | 127 | 19 |
| 9 | 11 | -1 | 0 | 41 | 1 | 22 | 6 | 0 | 0 | 43 | 1 | 7 | 3 | 1 | 379 | 378 | 4 | 3 | 21 | 1 | 0 | 6 | 1 | 8 | 16 | 2 | 69 | 82 | 68 |
| 11 | 11 | -1 | 72 | 55 | 34 | 0 | 8 | 0 | 700 | 711 | 6 | 9 | 3 | 1 | 802 | 812 | 13 | 5 | 21 | 1 | 0 | 28 | 1 | 10 | 16 | 2 | 58 | 11 | 57 |
| 13 | 11 | -1 | 30 | 18 | 29 | 2 | 8 | 0 | 190 | 208 | 5 | 11 | 3 | 1 | 110 | 103 | 26 | 9 | 21 | 1 | 0 | 54 | 1 | 14 | 16 | 2 | 0 | 45 | 1 |
| 15 | 11 | -1 | 0 | 2 | 1 | 4 | 8 | 0 | 455 | 465 | 9 | 13 | 3 | 1 | 70 | 76 | 35 | 11 | 21 | 1 | 0 | 18 | 1 | 16 | 16 | 2 | 0 | 28 | 1 |
| 17 | 11 | -1 | 0 | 22 | 1 | 6 | 8 | 0 | 717 | 649 | 9 | 15 | 3 | 1 | 96 | 113 | 27 | 1 | 23 | 1 | 0 | 49 | 1 | 0 | 18 | 2 | 0 | 63 | 1 |
| 19 | 11 | -1 | 124 | 121 | 11 | 8 | 8 | 0 | 265 | 279 | 5 | 17 | 3 | 1 | 90 | 107 | 38 | 3 | 23 | 1 | 0 | 17 | 1 | 2 | 18 | 2 | 89 | 80 | 51 |
| 3 | 13 | -1 | 195 | 216 | 13 | 10 | 8 | 0 | 256 | 229 | 10 | 19 | 3 | 1 | 0 | 36 | 1 | 5 | 23 | 1 | 74 | 13 | 73 | 4 | 18 | 2 | 55 | 17 | 54 |
| 5 | 13 | -1 | 373 | 389 | 7 | 12 | 8 | 0 | 140 | 144 | 13 | 21 | 3 | 1 | 38 | 26 | 38 | 7 | 23 | 1 | 0 | 36 | 1 | 6 | 18 | 2 | 70 | 82 | 70 |
| 7 | 13 | -1 | 102 | 123 | 22 | 14 | 8 | 0 | 102 | 111 | 35 | 1 | 5 | 1 | 1312 | 1376 | 9 | 1 | 25 | 1 | 0 | 30 | 1 | 8 | 18 | 2 | 0 | 26 | 1 |
| 9 | 13 | -1 | 114 | 136 | 52 | 16 | 8 | 0 | 39 | 13 | 39 | 3 | 5 | 1 | 486 | 550 | 6 | 0 | 2 | 2 | 2264 | 2179 | 5 | 10 | 18 | 2 | 39 | 42 | 38 |
| 11 | 13 | -1 | 101 | 105 | 36 | 18 | 8 | 0 | 0 | 41 | 1 | 5 | 5 | 1 | 613 | 680 | 13 | 2 | 2 | 2 | 2566 | 2533 | 5 | 12 | 18 | 2 | 37 | 29 | 36 |
| 13 | 13 | -1 | 66 | 57 | 65 | 20 | 8 | 0 | 19 | 9 | 19 | 7 | 5 | 1 | 303 | 315 | 5 | 4 | 2 | 2 | 693 | 697 | 8 | 14 | 18 | 2 | 0 | 17 | 1 |
| 15 | 13 | -1 | 31 | 29 | 31 | 2 | 10 | 0 | 785 | 745 | 20 | 9 | 5 | 1 | 176 | 176 | 11 | 6 | 2 | 2 | 302 | 339 | 5 | 2 | 20 | 2 | 25 | 21 | 24 |
| 17 | 13 | -1 | 0 | 25 | 1 | 4 | 10 | 0 | 1178 | 1232 | 9 | 11 | 5 | 1 | 122 | 141 | 11 | 8 | 2 | 2 | 298 | 291 | 6 | 4 | 20 | 2 | 66 | 62 | 65 |
| 19 | 13 | -1 | 0 | 15 | 1 | 6 | 10 | 0 | 164 | 168 | 9 | 13 | 5 | 1 | 70 | 48 | 44 | 10 | 2 | 2 | 252 | 233 | 8 | 6 | 20 | 2 | 0 | 26 | 1 |
| 1 | 15 | -1 | 123 | 116 | 29 | 8 | 10 | 0 | 214 | 196 | 10 | 15 | 5 | 1 | 0 | 67 | 1 | 12 | 2 | 2 | 87 | 68 | 23 | 8 | 20 | 2 | 0 | 66 | 1 |
| 3 | 15 | -1 | 290 | 291 | 16 | 10 | 10 | 0 | 86 | 31 | 20 | 17 | 5 | 1 | 32 | 22 | 31 | 14 | 2 | 2 | 0 | 103 | 1 | 10 | 20 | 2 | 33 | 35 | 33 |
| 5 | 15 | -1 | 224 | 226 | 10 | 12 | 10 | 0 | 131 | 136 | 16 | 19 | 5 | 1 | 81 | 13 | 80 | 16 | 2 | 2 | 0 | 58 | 1 | 12 | 20 | 2 | 0 | 6 | 1 |
| 7 | 15 | -1 | 177 | 173 | 11 | 14 | 10 | 0 | 0 | 38 | 1 | 21 | 5 | 1 | 48 | 29 | 47 | 18 | 2 | 2 | 65 | 85 | 64 | 0 | 22 | 2 | 56 | 41 | 55 |
| 9 | 15 | -1 | 115 | 97 | 74 | 16 | 10 | 0 | 0 | 33 | 1 | 1 | 7 | 1 | 855 | 871 | 6 | 20 | 2 | 2 | 47 | 22 | 47 | 2 | 22 | 2 | 54 | 26 | 54 |
| 11 | 15 | -1 | 66 | 70 | 65 | 18 | 10 | 0 | 69 | 11 | 68 | 3 | 7 | 1 | 1291 | 1321 | 5 | 22 | 2 | 2 | 0 | 4 | 1 | 4 | 22 | 2 | 0 | 17 | 1 |
| 13 | 15 | -1 | 0 | 19 | 1 | 20 | 10 | 0 | 59 | 57 | 59 | 5 | 7 | 1 | 550 | 515 | 6 | 2 | 4 | 2 | 1224 | 1201 | 22 | 6 | 22 | 2 | 0 | 5 | 1 |
| 15 | 15 | -1 | 0 | 40 | 1 | 0 | 12 | 0 | 182 | 182 | 10 | 7 | 7 | 1 | 96 | 92 | 11 | 4 | 4 | 2 | 76 | 78 | 15 | 8 | 22 | 2 | 0 | 18 | 1 |
| 17 | 15 | -1 | 0 | 5 | 1 | 2 | 12 | 0 | 0 | 95 | 1 | 9 | 7 | 1 | 154 | 162 | 9 | 6 | 4 | 2 | 359 | 355 | 4 | 10 | 22 | 2 | 0 | 22 | 1 |
| 1 | 17 | -1 | 202 | 201 | 11 | 4 | 12 | 0 | 225 | 218 | 7 | 11 | 7 | 1 | 321 | 317 | 10 | 8 | 4 | 2 | 528 | 502 | 5 | 2 | 24 | 2 | 0 | 24 | 1 |
| 3 | 17 | -1 | 46 | 30 | 45 | 6 | 12 | 0 | 423 | 456 | 14 | 13 | 7 | 1 | 76 | 83 | 39 | 10 | 4 | 2 | 168 | 152 | 7 | 4 | 24 | 2 | 0 | 28 | 1 |
| 5 | 17 | -1 | 0 | 46 | 1 | 8 | 12 | 0 | 56 | 19 | 56 | 15 | 7 | 1 | 98 | 124 | 98 | 12 | 4 | 2 | 79 | 79 | 78 | 6 | 24 | 2 | 0 | 26 | 1 |
| 7 | 17 | -1 | 136 | 138 | 16 | 10 | 12 | 0 | 134 | 140 | 66 | 17 | 7 | 1 | 0 | 57 | 1 | 14 | 4 | 2 | 66 | 89 | 53 | 1 | 3 | 3 | 794 | 771 | 7 |
| 9 | 17 | -1 | 50 | | | | | | | | | | | | | | | | | | | | | | | | | | |

Table 10. Observed and calculated structure factors for pchcl7a

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| 15 | 7 | 3 | 140 | 136 | 15 | 18 | 6 | 4 | 43 | 52 | 43 | 9 | 7 | 5 | 298 | 283 | 5 | 14 | 8 | 6 | 44 | 56 | 44 | 1 | 13 | 7 | 153 | 124 | 21 | 17 | 7 | 3 | 0 | 30 | 1 | 20 | 6 | 4 | 32 | 21 | 32 | 11 | 7 | 5 | 287 | 272 | 15 | 16 | 8 | 6 | 101 | 115 | 29 | 3 | 13 | 7 | 165 | 174 | 11 | 19 | 7 | 3 | 68 | 9 | 68 | 0 | 8 | 4 | 597 | 599 | 9 | 13 | 7 | 5 | 82 | 104 | 82 | 18 | 8 | 6 | 0 | 22 | 1 | 5 | 13 | 7 | 179 | 179 | 14 | 21 | 7 | 3 | 0 | 13 | 1 | 2 | 8 | 4 | 488 | 525 | 12 | 15 | 7 | 5 | 145 | 146 | 16 | 20 | 8 | 6 | 43 | 13 | 42 | 7 | 13 | 7 | 134 | 145 | 16 | 1 | 9 | 3 | 549 | 538 | 7 | 4 | 8 | 4 | 76 | 73 | 14 | 17 | 7 | 5 | 0 | 52 | 1 | 0 | 10 | 6 | 243 | 205 | 10 | 9 | 13 | 7 | 0 | 12 | 1 | 11 | 13 | 7 | 0 | 73 | 1 | 3 | 9 | 3 | 383 | 388 | 5 | 6 | 8 | 4 | 103 | 101 | 10 | 19 | 7 | 5 | 0 | 13 | 1 | 4 | 10 | 6 | 116 | 134 | 11 | 13 | 13 | 7 | 0 | 18 | 1 | 5 | 9 | 3 | 302 | 283 | 7 | 8 | 8 | 4 | 149 | 118 | 9 | 21 | 7 | 5 | 73 | 37 | 73 | 2 | 10 | 6 | 0 | 12 | 1 | 11 | 13 | 7 | 0 | 73 | 1 | 7 | 9 | 3 | 182 | 197 | 7 | 10 | 8 | 4 | 118 | 104 | 20 | 19 | 7 | 5 | 0 | 13 | 1 | 4 | 10 | 6 | 121 | 108 | 13 | 15 | 13 | 7 | 71 | 27 | 70 | 1 | 9 | 3 | 93 | 88 | 31 | 12 | 8 | 4 | 156 | 158 | 14 | 3 | 9 | 5 | 162 | 151 | 7 | 8 | 10 | 6 | 123 | 142 | 59 | 17 | 13 | 7 | 54 | 33 | 54 | 11 | 9 | 3 | 62 | 22 | 62 | 14 | 8 | 4 | 107 | 94 | 17 | 5 | 9 | 5 | 0 | 43 | 1 | 10 | 10 | 6 | 125 | 144 | 16 | 1 | 15 | 7 | 78 | 90 | 78 | 13 | 9 | 3 | 64 | 118 | 64 | 16 | 8 | 4 | 53 | 53 | 53 | 7 | 9 | 5 | 212 | 207 | 7 | 12 | 10 | 6 | 0 | 29 | 1 | 3 | 15 | 7 | 25 | 50 | 24 | 17 | 9 | 3 | 0 | 67 | 1 | 18 | 8 | 4 | 71 | 59 | 70 | 9 | 9 | 5 | 190 | 197 | 10 | 14 | 10 | 6 | 0 | 39 | 1 | 5 | 15 | 7 | 51 | 63 | 50 | 15 | 9 | 3 | 56 | 35 | 55 | 20 | 8 | 4 | 42 | 6 | 42 | 11 | 9 | 5 | 73 | 60 | 31 | 16 | 10 | 6 | 0 | 18 | 1 | 7 | 15 | 7 | 77 | 67 | 32 | 19 | 9 | 3 | 0 | 21 | 1 | 2 | 10 | 4 | 296 | 277 | 15 | 13 | 9 | 5 | 54 | 35 | 53 | 18 | 10 | 6 | 0 | 57 | 1 | 9 | 15 | 7 | 49 | 30 | 49 | 1 | 1 | 11 | 3 | 215 | 205 | 7 | 4 | 10 | 4 | 138 | 133 | 9 | 15 | 9 | 5 | 123 | 103 | 20 | 2 | 12 | 6 | 91 | 59 | 90 | 11 | 15 | 7 | 42 | 31 | 41 | 3 | 11 | 3 | 63 | 52 | 21 | 6 | 10 | 4 | 215 | 196 | 6 | 17 | 9 | 5 | 76 | 70 | 76 | 4 | 12 | 6 | 110 | 132 | 15 | 13 | 15 | 7 | 0 | 27 | 1 | 5 | 11 | 3 | 82 | 45 | 15 | 8 | 10 | 4 | 463 | 440 | 5 | 19 | 9 | 5 | 0 | 15 | 1 | 6 | 12 | 6 | 0 | 98 | 1 | 15 | 15 | 7 | 0 | 19 | 1 | 7 | 11 | 3 | 171 | 170 | 9 | 10 | 10 | 4 | 0 | 95 | 1 | 8 | 12 | 6 | 242 | 212 | 19 | 1 | 17 | 7 | 0 | 15 | 1 | 9 | 11 | 3 | 179 | 178 | 10 | 12 | 10 | 4 | 83 | 106 | 73 | 3 | 11 | 3 | 0 | 34 | 1 | 5 | 11 | 5 | 69 | 16 | 20 | 12 | 12 | 6 | 0 | 50 | 1 | 5 | 17 | 7 | 0 | 86 | 1 | 11 | 11 | 3 | 140 | 133 | 14 | 14 | 10 | 4 | 0 | 87 | 1 | 7 | 11 | 5 | 200 | 217 | 12 | 14 | 12 | 6 | 24 | 20 | 24 | 7 | 17 | 7 | 81 | 65 | 81 | 15 | 11 | 3 | 39 | 34 | 38 | 16 | 10 | 4 | 0 | 13 | 1 | 9 | 11 | 5 | 285 | 285 | 15 | 16 | 12 | 6 | 93 | 115 | 93 | 9 | 17 | 7 | 45 | 45 | 45 | 17 | 11 | 3 | 45 | 29 | 44 | 20 | 10 | 4 | 0 | 11 | 1 | 11 | 11 | 5 | 0 | 49 | 1 | 18 | 12 | 6 | 0 | 20 | 1 | 11 | 17 | 7 | 0 | 34 | 1 | 19 | 11 | 3 | 24 | 26 | 23 | 0 | 12 | 4 | 462 | 417 | 8 | 13 | 11 | 5 | 76 | 49 | 54 | 0 | 14 | 6 | 321 | 323 | 11 | 13 | 17 | 7 | 0 | 28 | 1 | 1 | 13 | 3 | 194 | 194 | 8 | 2 | 12 | 4 | 97 | 96 | 14 | 15 | 11 | 5 | 63 | 40 | 62 | 2 | 14 | 6 | 211 | 208 | 9 | 1 | 19 | 7 | 26 | 21 | 25 | 3 | 13 | 3 | 57 | 70 | 56 | 4 | 12 | 4 | 32 | 44 | 32 | 17 | 11 | 5 | 91 | 78 | 39 | 4 | 14 | 6 | 74 | 88 | 43 | 3 | 19 | 7 | 73 | 50 | 73 | 5 | 13 | 3 | 150 | 125 | 89 | 6 | 12 | 4 | 200 | 217 | 9 | 19 | 11 | 5 | 0 | 14 | 1 | 6 | 14 | 6 | 156 | 141 | 44 | 5 | 19 | 7 | 105 | 100 | 29 | 7 | 13 | 3 | 266 | 264 | 22 | 8 | 12 | 4 | 130 | 102 | 14 | 1 | 13 | 5 | 240 | 220 | 8 | 8 | 14 | 6 | 0 | 31 | 1 | 7 | 19 | 7 | 0 | 18 | 1 | 9 | 13 | 3 | 82 | 89 | 26 | 10 | 12 | 4 | 114 | 114 | 18 | 3 | 13 | 5 | 123 | 112 | 14 | 10 | 14 | 6 | 0 | 41 | 1 | 9 | 19 | 7 | 0 | 16 | 1 | 11 | 13 | 3 | 0 | 29 | 1 | 12 | 12 | 4 | 67 | 59 | 66 | 5 | 13 | 5 | 49 | 45 | 49 | 12 | 14 | 6 | 68 | 34 | 67 | 11 | 13 | 3 | 0 | 43 | 1 | 14 | 12 | 4 | 42 | 29 | 41 | 7 | 13 | 5 | 275 | 286 | 8 | 14 | 14 | 6 | 0 | 13 | 1 | 14 | 14 | 6 | 0 | 13 | 1 | 7 | 19 | 7 | 0 | 18 | 1 | 15 | 13 | 3 | 0 | 24 | 1 | 16 | 12 | 4 | 13 | 23 | 12 | 9 | 13 | 5 | 185 | 187 | 11 | 16 | 14 | 6 | 70 | 13 | 69 | 3 | 21 | 7 | 86 | 71 | 70 | 15 | 13 | 3 | 0 | 11 | 1 | 18 | 12 | 4 | 0 | 35 | 1 | 11 | 13 | 5 | 43 | 40 | 43 | 2 | 16 | 6 | 0 | 87 | 1 | 5 | 21 | 7 | 71 | 38 | 70 | 19 | 13 | 3 | 0 | 6 | 1 | 2 | 14 | 4 | 115 | 111 | 15 | 13 | 13 | 5 | 46 | 24 | 45 | 4 | 16 | 6 | 116 | 96 | 33 | 7 | 21 | 7 | 0 | 8 | 1 | 1 | 15 | 3 | 186 | 172 | 10 | 4 | 14 | 4 | 246 | 232 | 8 | 15 | 13 | 5 | 0 | 35 | 1 | 6 | 16 | 6 | 123 | 126 | 19 | 9 | 21 | 7 | 18 | 5 | 18 | 3 | 15 | 3 | 90 | 68 | 21 | 6 | 14 | 4 | 160 | 147 | 12 | 17 | 13 | 5 | 0 | 35 | 1 | 1 | 15 | 5 | 76 | 52 | 76 | 8 | 16 | 6 | 64 | 59 | 64 | 1 | 23 | 7 | 0 | 19 | 1 | 5 | 15 | 3 | 120 | 121 | 22 | 8 | 14 | 4 | 220 | 221 | 10 | 1 | 15 | 5 | 78 | 65 | 46 | 10 | 16 | 6 | 0 | 94 | 1 | 3 | 23 | 7 | 0 | 19 | 1 | 7 | 15 | 3 | 117 | 122 | 18 | 10 | 14 | 4 | 0 | 73 | 1 | 5 | 15 | 5 | 180 | 174 | 19 | 12 | 16 | 6 | 0 | 31 | 1 | 0 | 8 | 8 | 68 | 132 | 67 | 9 | 15 | 3 | 0 | 29 | 1 | 12 | 14 | 4 | 60 | 37 | 60 | 5 | 13 | 5 | 139 | 134 | 14 | 14 | 16 | 6 | 0 | 30 | 1 | 2 | 8 | 8 | 202 | 200 | 6 | 11 | 15 | 3 | 0 | 44 | 1 | 16 | 14 | 4 | 41 | 37 | 41 | 9 | 15 | 5 | 34 | 44 | 34 | 16 | 16 | 6 | 0 | 30 | 1 | 4 | 8 | 8 | 0 | 51 | 1 | 13 | 15 | 3 | 30 | 15 | 30 | 18 | 14 | 4 | 31 | 32 | 31 | 11 | 15 | 5 | 0 | 54 | 1 | 2 | 18 | 6 | 0 | 107 | 1 | 8 | 8 | 8 | 0 | 41 | 1 | 15 | 15 | 3 | 47 | 19 | 47 | 18 | 14 | 4 | 41 | 37 | 41 | 13 | 15 | 5 | 44 | 41 | 44 | 4 | 18 | 6 | 81 | 57 | 39 | 10 | 8 | 8 | 0 | 91 | 1 | 17 | 15 | 3 | 0 | 69 | 1 | 2 | 16 | 4 | 116 | 113 | 41 | 15 | 15 | 5 | 68 | 31 | 68 | 6 | 18 | 6 | 75 | 83 | 75 | 12 | 8 | 8 | 78 | 36 | 45 | 3 | 17 | 3 | 52 | 27 | 52 | 4 | 16 | 4 | 59 | 84 | 58 | 17 | 15 | 5 | 65 | 43 | 65 | 8 | 18 | 6 | 0 | 18 | 1 | 14 | 8 | 8 | 68 | 7 | 67 | 5 | 17 | 3 | 75 | 65 | 58 | 6 | 16 | 4 | 114 | 117 | 39 | 1 | 17 | 5 | 0 | 47 | 1 | 10 | 18 | 6 | 40 | 28 | 40 | 16 | 8 | 8 | 0 | 23 | 1 | 7 | 17 | 3 | 67 | 35 | 67 | 8 | 16 | 4 | 0 | 40 | 1 | 3 | 17 | 5 | 101 | 90 | 38 | 12 | 18 | 6 | 0 | 43 | 1 | 18 | 8 | 8 | 0 | 21 | 1 | 9 | 17 | 3 | 49 | 53 | 49 | 10 | 16 | 4 | 36 | 7 | 35 | 5 | 17 | 5 | 0 | 135 | 1 | 14 | 18 | 6 | 108 | 12 | 50 | 2 | 10 | 8 | 90 | 104 | 23 | 11 | 17 | 3 | 32 | 42 | 31 | 12 | 16 | 4 | 0 | 36 | 1 | 7 | 17 | 5 | 112 | 105 | 34 | 2 | 20 | 6 | 0 | 25 | 1 | 4 | 10 | 8 | 195 | 187 | 13 | 13 | 17 | 3 | 48 | 37 | 47 | 14 | 16 | 4 | 0 | 44 | 1 | 9 | 17 | 5 | 0 | 50 | 1 | 4 | 20 | 6 | 109 | 106 | 28 | 6 | 10 | 8 | 209 | 198 | 12 | 15 | 17 | 3 | 63 | 25 | 63 | 16 | 16 | 4 | 70 | 9 | 70 | 11 | 17 | 5 | 106 | 70 | 27 | 6 | 20 | 6 | 0 | 73 | 1 | 8 | 10 | 8 | 147 | 151 | 13 | 1 | 19 | 3 | 0 | 31 | 1 | 2 | 18 | 4 | 64 | 48 | 64 | 13 | 17 | 5 | 0 | 24 | 1 | 8 | 20 | 6 | 0 | 22 | 1 | 10 | 10 | 8 | 25 | 25 | 24 | 3 | 19 | 3 | 40 | 33 | 39 | 4 | 18 | 4 | 0 | 78 | 1 | 15 | 17 | 5 | 0 | 33 | 1 | 10 | 20 | 6 | 61 | 51 | 60 | 12 | 10 | 8 | 49 | 58 | 49 | 5 | 19 | 3 | 79 | 76 | 42 | 6 | 18 | 4 | 0 | 54 | 1 | 0 | 22 | 6 | 28 | 24 | 27 | 14 | 10 | 8 | 54 | 22 | 53 | 7 | 19 | 3 | 0 | 26 | 1 | 8 | 18 | 4 | 0 | 32 | 1 | 3 | 19 | 5 | 39 | 22 | 38 | 2 | 22 | 6 | 40 | 25 | 40 | 16 | 10 | 8 | 61 | 28 | 61 | 1 | 1 | 9 | 3 | 68 | 28 | 68 | 10 | 18 | 4 | 37 | 45 | 36 | 5 | 19 | 5 | 90 | 105 | 47 | 4 | 22 | 6 | 0 | 44 | 1 | 18 | 10 | 8 | 0 | 4 | 2 | 11 | 13 | 3 | 0 | 22 | 1 | 12 | 18 | 4 | 27 | 30 | 26 | 7 | 19 | 5 | 27 | 6 | 26 | 6 | 22 | 6 | 75 | 21 | 74 | 0 | 12 | 8 | 100 | 92 | 26 | 13 | 19 | 3 | 38 | 16 | 38 | 14 | 18 | 4 | 0 | 29 | 1 | 8 | 22 | 6 | 35 | 20 | 35 | 2 | 12 | 8 | 206 | 170 | 18 | 1 | 21 | 3 | 0 | 9 | 1 | 0 | 20 | 4 | 0 | 12 | 1 | 1 | 19 | 5 | 27 | 23 | 27 | 1 | 7 | 7 | 454 | 514 | 6 | 4 | 12 | 8 | 106 | 82 | 18 | 3 | 21 | 3 | 0 | 33 | 1 | 13 | 19 | 5 | 33 | 44 | 32 | 3 | 7 | 7 | 290 | 291 | 12 | 6 | 12 | 8 | 31 | 21 | 31 | 5 | 21 | 3 | 34 | 30 | 34 | 4 | 20 | 4 | 51 | 34 | 51 | 1 | 21 | 5 | 53 | 12 | 53 | 5 | 7 | 7 | 210 | 206 | 7 | 8 | 12 | 8 | 51 | 45 | 50 | 7 | 21 | 3 | 80 | 42 | 79 | 6 | 20 | 4 | 0 | 51 | 1 | 3 | 21 | 5 | 74 | 79 | 65 | 7 | 7 | 7 | 131 | 164 |

Table 10. Observed and calculated structure factors for pchcl7a

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|----|----|---|------|------|-----|----|----|----|------|------|-----|----|----|----|------|------|-----|----|----|----|------|------|-----|----|----|----|------|------|-----|
| 0 | 20 | 8 | 0 | 34 | 1 | 3 | 15 | 9 | 58 | 46 | 58 | 12 | 12 | 10 | 0 | 34 | 1 | 3 | 13 | 11 | 76 | 71 | 75 | 0 | 16 | 12 | 0 | 17 | 1 |
| 2 | 20 | 8 | 25 | 15 | 24 | 5 | 15 | 9 | 27 | 7 | 27 | 14 | 12 | 10 | 58 | 19 | 58 | 5 | 13 | 11 | 147 | 125 | 20 | 2 | 16 | 12 | 0 | 12 | 1 |
| 4 | 20 | 8 | 0 | 41 | 1 | 7 | 15 | 9 | 0 | 69 | 1 | 16 | 12 | 10 | 0 | 24 | 1 | 7 | 13 | 11 | 0 | 32 | 1 | 4 | 16 | 12 | 0 | 23 | 1 |
| 6 | 20 | 8 | 44 | 24 | 44 | 9 | 15 | 9 | 55 | 9 | 55 | 0 | 14 | 10 | 79 | 30 | 45 | 9 | 13 | 11 | 46 | 14 | 45 | 6 | 16 | 12 | 88 | 74 | 88 |
| 8 | 20 | 8 | 0 | 21 | 1 | 11 | 15 | 9 | 0 | 29 | 1 | 2 | 14 | 10 | 70 | 53 | 70 | 11 | 13 | 11 | 0 | 17 | 1 | 8 | 16 | 12 | 51 | 25 | 51 |
| 10 | 20 | 8 | 0 | 11 | 1 | 13 | 15 | 9 | 0 | 18 | 1 | 4 | 14 | 10 | 42 | 62 | 41 | 13 | 13 | 11 | 0 | 30 | 1 | 10 | 16 | 12 | 0 | 26 | 1 |
| 2 | 22 | 8 | 74 | 19 | 73 | 1 | 17 | 9 | 51 | 31 | 50 | 6 | 14 | 10 | 87 | 64 | 87 | 1 | 15 | 11 | 66 | 23 | 65 | 2 | 18 | 12 | 35 | 38 | 35 |
| 4 | 22 | 8 | 45 | 38 | 45 | 3 | 17 | 9 | 40 | 48 | 39 | 8 | 14 | 10 | 19 | 31 | 19 | 3 | 15 | 11 | 0 | 66 | 1 | 4 | 18 | 12 | 56 | 19 | 56 |
| 1 | 9 | 9 | 162 | 166 | 18 | 5 | 17 | 9 | 38 | 32 | 38 | 10 | 14 | 10 | 46 | 14 | 45 | 5 | 15 | 11 | 85 | 97 | 84 | 6 | 18 | 12 | 0 | 41 | 1 |
| 3 | 9 | 9 | 278 | 266 | 7 | 7 | 17 | 9 | 0 | 34 | 1 | 12 | 14 | 10 | 79 | 32 | 79 | 7 | 15 | 11 | 83 | 75 | 82 | 1 | 13 | 13 | 0 | 12 | 1 |
| 5 | 9 | 9 | 161 | 138 | 24 | 9 | 17 | 9 | 0 | 26 | 1 | 14 | 14 | 10 | 68 | 24 | 68 | 9 | 15 | 11 | 0 | 18 | 1 | 3 | 13 | 13 | 0 | 16 | 1 |
| 7 | 9 | 9 | 111 | 114 | 17 | 11 | 17 | 9 | 0 | 21 | 1 | 2 | 16 | 10 | 0 | 53 | 1 | 11 | 15 | 11 | 0 | 20 | 1 | 5 | 13 | 13 | 0 | 35 | 1 |
| 9 | 9 | 9 | 0 | 35 | 1 | 13 | 17 | 9 | 76 | 21 | 76 | 4 | 16 | 10 | 0 | 66 | 1 | 1 | 17 | 11 | 0 | 41 | 1 | 7 | 13 | 13 | 0 | 19 | 1 |
| 11 | 9 | 9 | 0 | 12 | 1 | 1 | 19 | 9 | 0 | 49 | 1 | 6 | 16 | 10 | 73 | 69 | 73 | 3 | 17 | 11 | 0 | 24 | 1 | 9 | 13 | 13 | 0 | 10 | 1 |
| 13 | 9 | 9 | 0 | 26 | 1 | 3 | 19 | 9 | 0 | 36 | 1 | 8 | 16 | 10 | 0 | 56 | 1 | 5 | 17 | 11 | 89 | 45 | 88 | 11 | 13 | 13 | 0 | 23 | 1 |
| 15 | 9 | 9 | 0 | 22 | 1 | 5 | 19 | 9 | 27 | 21 | 26 | 10 | 16 | 10 | 0 | 16 | 1 | 7 | 17 | 11 | 56 | 65 | 55 | 1 | 15 | 13 | 39 | 10 | 38 |
| 17 | 9 | 9 | 81 | 22 | 81 | 7 | 19 | 9 | 17 | 13 | 16 | 12 | 16 | 10 | 0 | 20 | 1 | 9 | 17 | 11 | 59 | 51 | 59 | 3 | 15 | 13 | 54 | 27 | 54 |
| 1 | 11 | 9 | 70 | 65 | 24 | 9 | 19 | 9 | 0 | 42 | 1 | 0 | 18 | 10 | 67 | 60 | 67 | 1 | 19 | 11 | 86 | 50 | 43 | 5 | 15 | 13 | 0 | 29 | 1 |
| 3 | 11 | 9 | 173 | 153 | 12 | 1 | 21 | 9 | 0 | 26 | 1 | 2 | 18 | 10 | 0 | 35 | 1 | 3 | 19 | 11 | 0 | 36 | 1 | 7 | 15 | 13 | 88 | 49 | 39 |
| 5 | 11 | 9 | 210 | 207 | 17 | 3 | 21 | 9 | 0 | 17 | 1 | 4 | 18 | 10 | 0 | 31 | 1 | 5 | 19 | 11 | 0 | 30 | 1 | 9 | 15 | 13 | 29 | 43 | 29 |
| 7 | 11 | 9 | 44 | 51 | 44 | 5 | 21 | 9 | 0 | 12 | 1 | 6 | 18 | 10 | 0 | 54 | 1 | 7 | 19 | 11 | 0 | 45 | 1 | 1 | 17 | 13 | 0 | 29 | 1 |
| 9 | 11 | 9 | 0 | 19 | 1 | 0 | 10 | 10 | 0 | 44 | 1 | 8 | 18 | 10 | 0 | 37 | 1 | 0 | 12 | 12 | 0 | 77 | 1 | 3 | 17 | 13 | 25 | 6 | 25 |
| 11 | 11 | 9 | 75 | 52 | 35 | 2 | 10 | 10 | 249 | 257 | 9 | 10 | 18 | 10 | 0 | 34 | 1 | 2 | 12 | 12 | 0 | 14 | 1 | 5 | 17 | 13 | 0 | 28 | 1 |
| 13 | 11 | 9 | 48 | 49 | 48 | 4 | 10 | 10 | 165 | 142 | 20 | 2 | 20 | 10 | 0 | 50 | 1 | 4 | 12 | 12 | 33 | 41 | 32 | 7 | 17 | 13 | 47 | 10 | 46 |
| 15 | 11 | 9 | 23 | 24 | 23 | 6 | 10 | 10 | 94 | 87 | 49 | 4 | 20 | 10 | 0 | 20 | 1 | 6 | 12 | 12 | 72 | 62 | 72 | 0 | 14 | 14 | 0 | 20 | 1 |
| 17 | 11 | 9 | 0 | 23 | 1 | 8 | 10 | 10 | 60 | 35 | 60 | 6 | 20 | 10 | 47 | 18 | 47 | 8 | 12 | 12 | 39 | 12 | 38 | 2 | 14 | 14 | 0 | 20 | 1 |
| 1 | 13 | 9 | 77 | 54 | 30 | 10 | 10 | 10 | 0 | 40 | 1 | 1 | 11 | 11 | 94 | 87 | 24 | 10 | 12 | 12 | 0 | 10 | 1 | 4 | 14 | 14 | 0 | 2 | 1 |
| 3 | 13 | 9 | 119 | 119 | 17 | 12 | 10 | 10 | 0 | 58 | 1 | 3 | 11 | 11 | 92 | 100 | 91 | 12 | 12 | 12 | 84 | 28 | 83 | 6 | 14 | 14 | 0 | 13 | 1 |
| 5 | 13 | 9 | 0 | 81 | 1 | 14 | 10 | 10 | 0 | 22 | 1 | 5 | 11 | 11 | 144 | 136 | 16 | 14 | 12 | 12 | 0 | 25 | 1 | 8 | 14 | 14 | 0 | 14 | 1 |
| 7 | 13 | 9 | 65 | 43 | 64 | 16 | 10 | 10 | 0 | 6 | 1 | 7 | 11 | 11 | 24 | 21 | 23 | 2 | 14 | 12 | 49 | 30 | 48 | 2 | 16 | 14 | 0 | 13 | 1 |
| 9 | 13 | 9 | 28 | 10 | 28 | 2 | 12 | 10 | 50 | 83 | 50 | 9 | 11 | 11 | 0 | 22 | 1 | 4 | 14 | 12 | 0 | 80 | 1 | 4 | 16 | 14 | 0 | 19 | 1 |
| 11 | 13 | 9 | 52 | 33 | 52 | 4 | 12 | 10 | 199 | 204 | 10 | 11 | 11 | 11 | 0 | 50 | 1 | 6 | 14 | 12 | 67 | 67 | 67 | 6 | 16 | 14 | 33 | 7 | 32 |
| 13 | 13 | 9 | 0 | 19 | 1 | 6 | 12 | 10 | 73 | 59 | 34 | 13 | 11 | 11 | 44 | 38 | 43 | 8 | 14 | 12 | 48 | 31 | 48 | 1 | 15 | 15 | 0 | 18 | 1 |
| 15 | 13 | 9 | 0 | 19 | 1 | 8 | 12 | 10 | 0 | 29 | 1 | 15 | 11 | 11 | 0 | 16 | 1 | 10 | 14 | 12 | 0 | 15 | 1 | 3 | 15 | 15 | 0 | 9 | 1 |
| 1 | 15 | 9 | 0 | 49 | 1 | 10 | 12 | 10 | 0 | 20 | 1 | 1 | 13 | 11 | 78 | 68 | 77 | 12 | 14 | 12 | 0 | 17 | 1 | | | | | | |

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