

SUPPORTING INFORMATION FOR

13-Methyl-2,6-dithia[7]metacyclophane - A useful molecule to connect VT NMR results and structure with calculations

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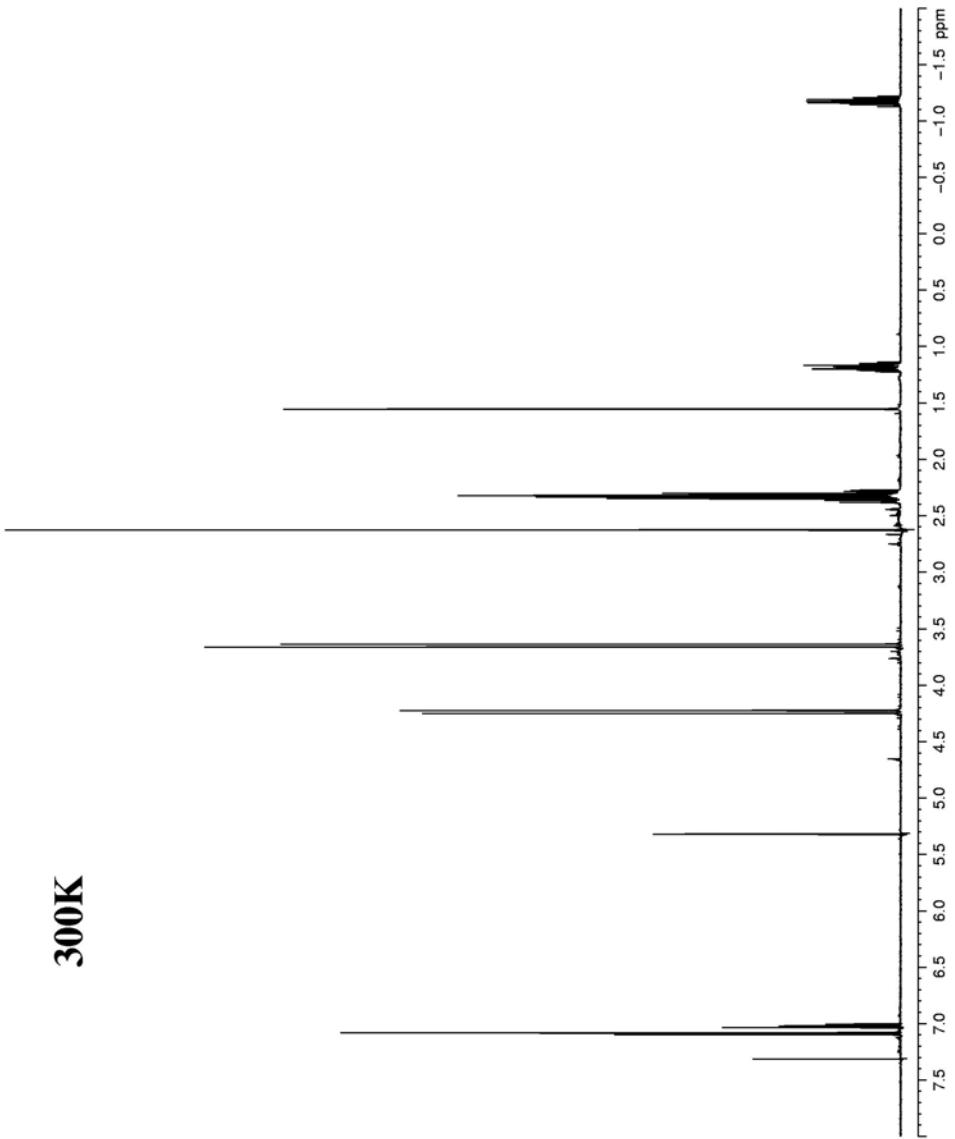
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CONTENTS

¹ H NMR spectrum of 1 at 300, 270, 260, 250, 240, 230, 220, 210, 205, 200, 190, 180, 175K in 3:1 CD ₂ Cl ₂ :CDCl ₃ at 500 MHz	3-15
¹³ C NMR spectrum of 1 at 300, 270, 250, 240, 230, 220, 210, 205, 200, 190, 180, 175K in 3:1 CD ₂ Cl ₂ :CDCl ₃ at 126 MHz	16-27
¹ H NMR spectrum of 2 at 300, 270, 260, 250, 240, 230, 220, 215, 210, 205, 200, 195, 190, 185, 180, 175K in 3:1 CD ₂ Cl ₂ :CDCl ₃ at 500 MHz	28-43
¹³ C NMR spectrum of 2 at 300, 220, 190, 180, in 3:1 CD ₂ Cl ₂ :CDCl ₃ at 126 MHz	44-47

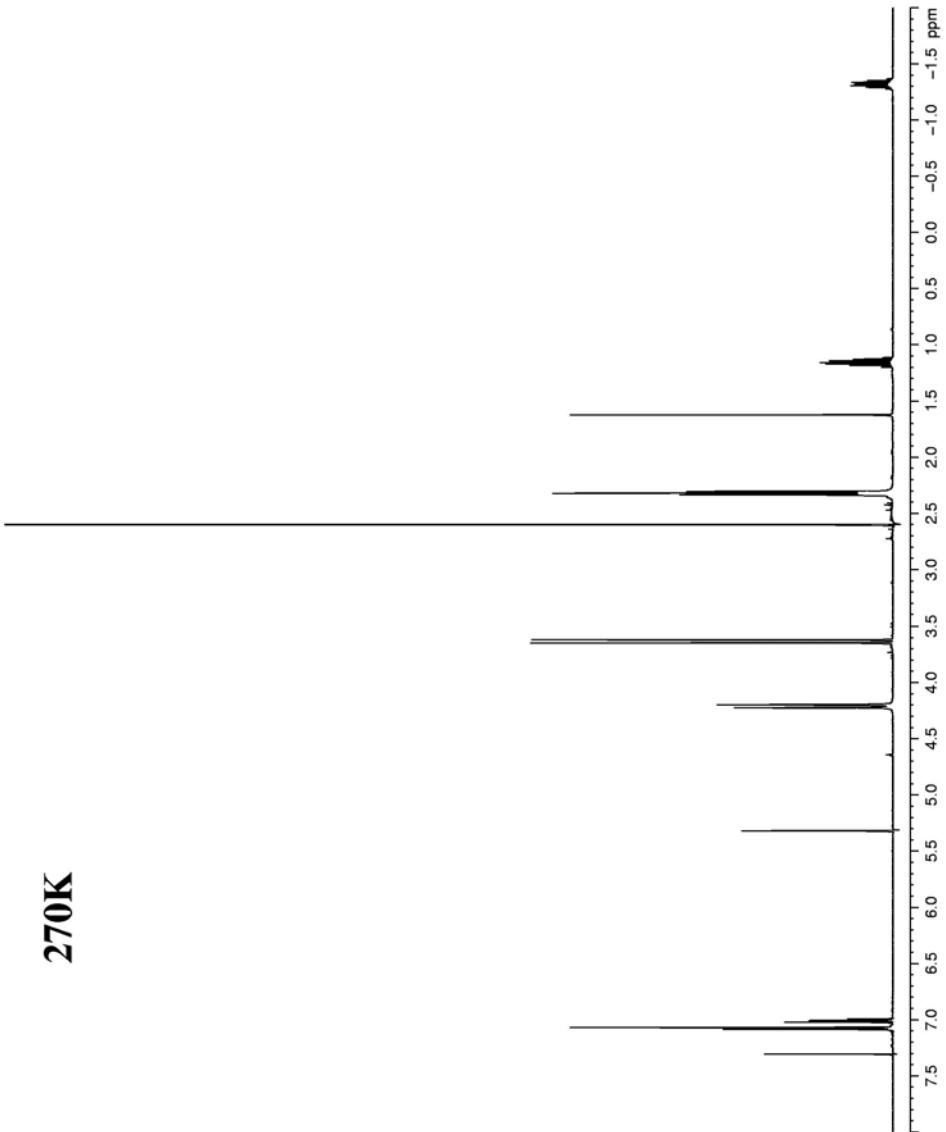
S(I)3

^1H NMR spectrum of **1** at 300K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$



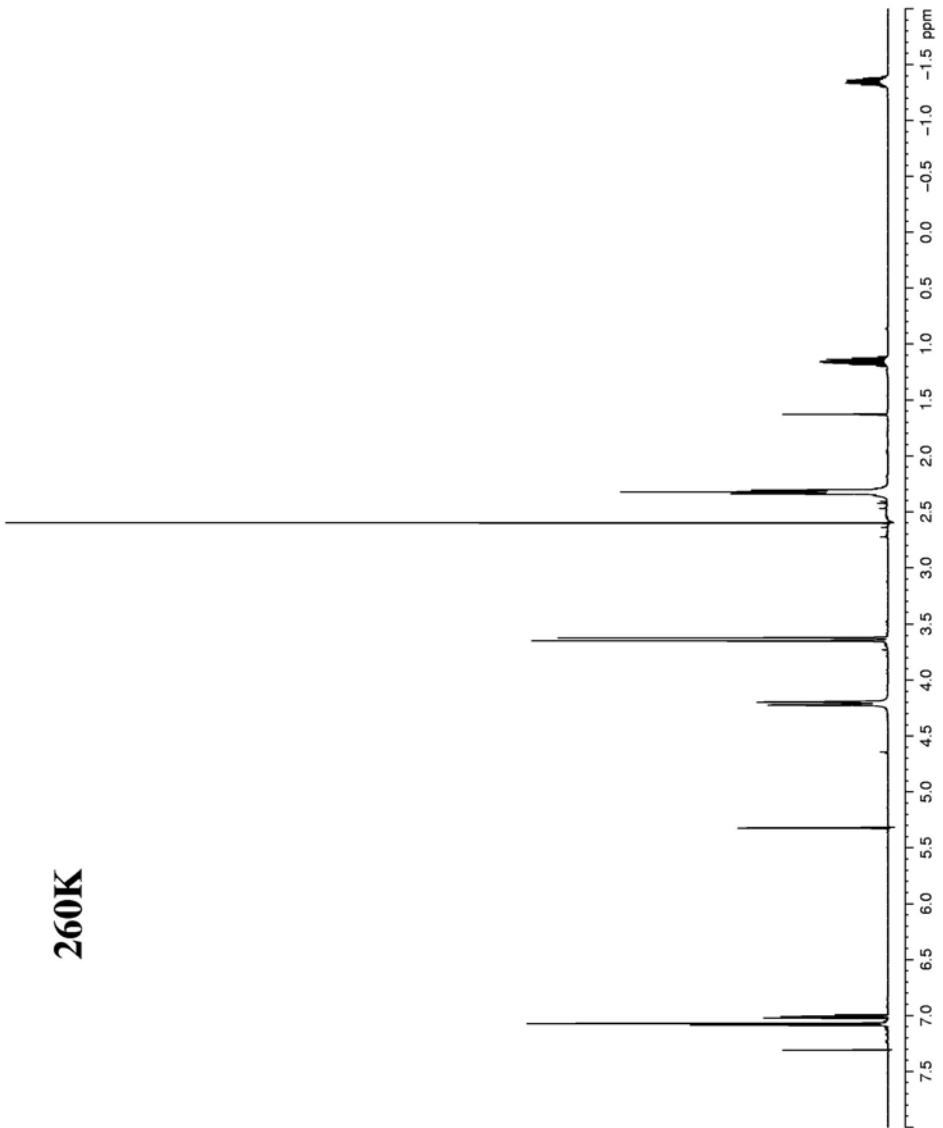
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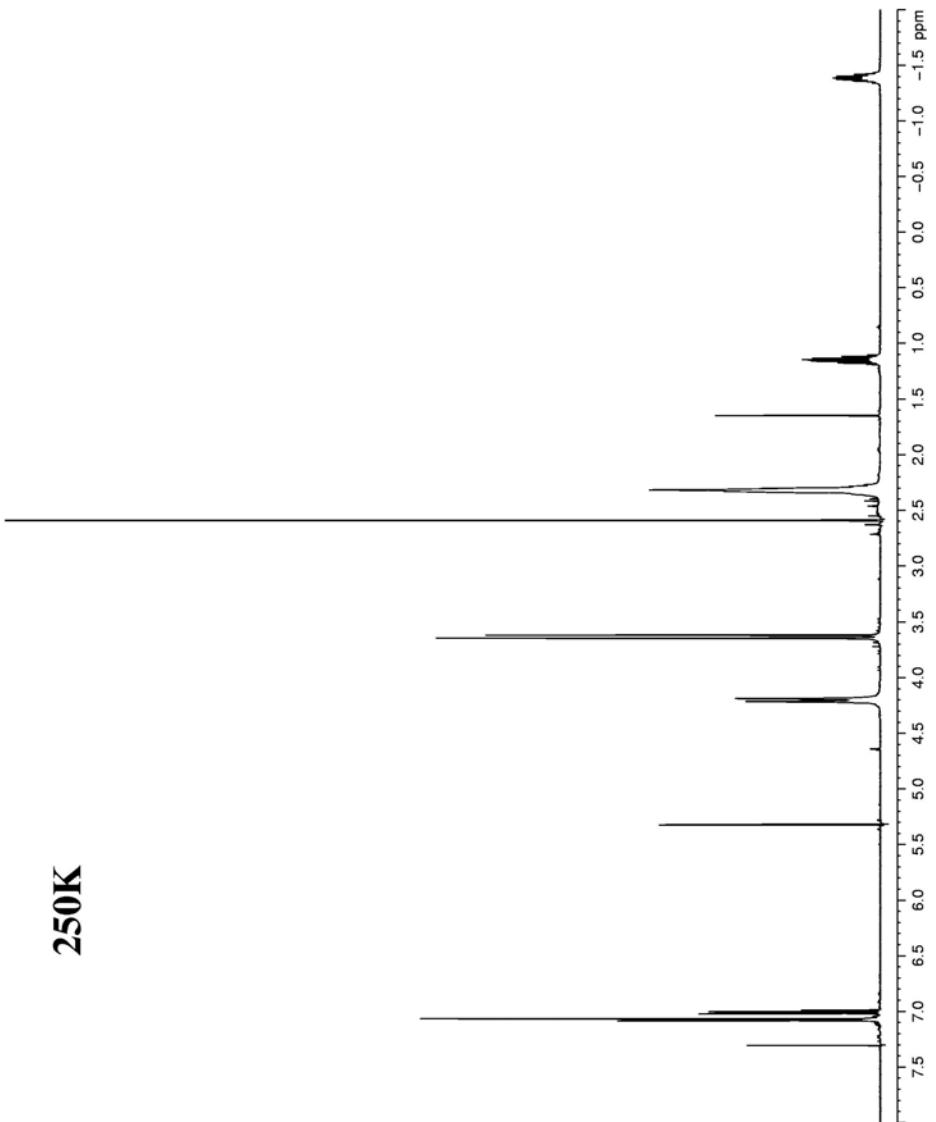


S(I)5

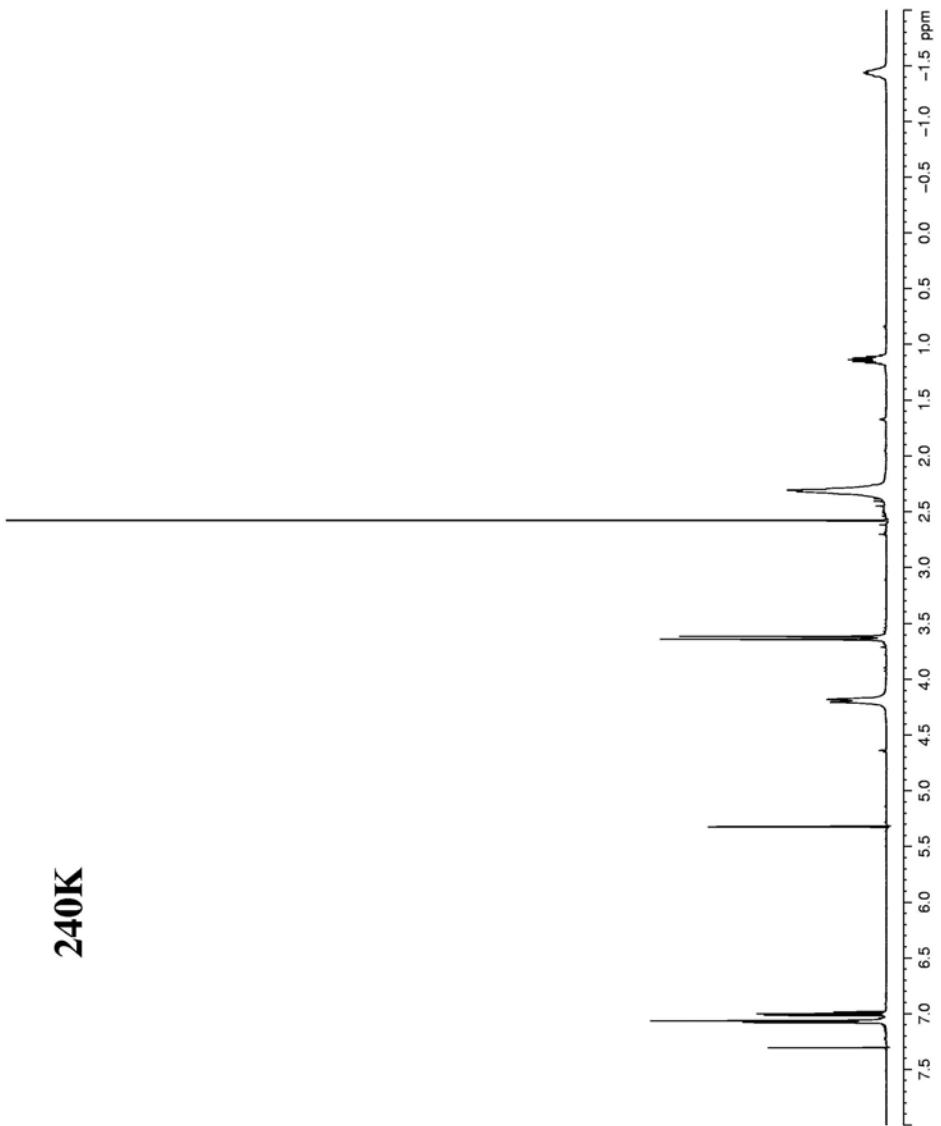
^1H NMR spectrum of **1** at 260K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$



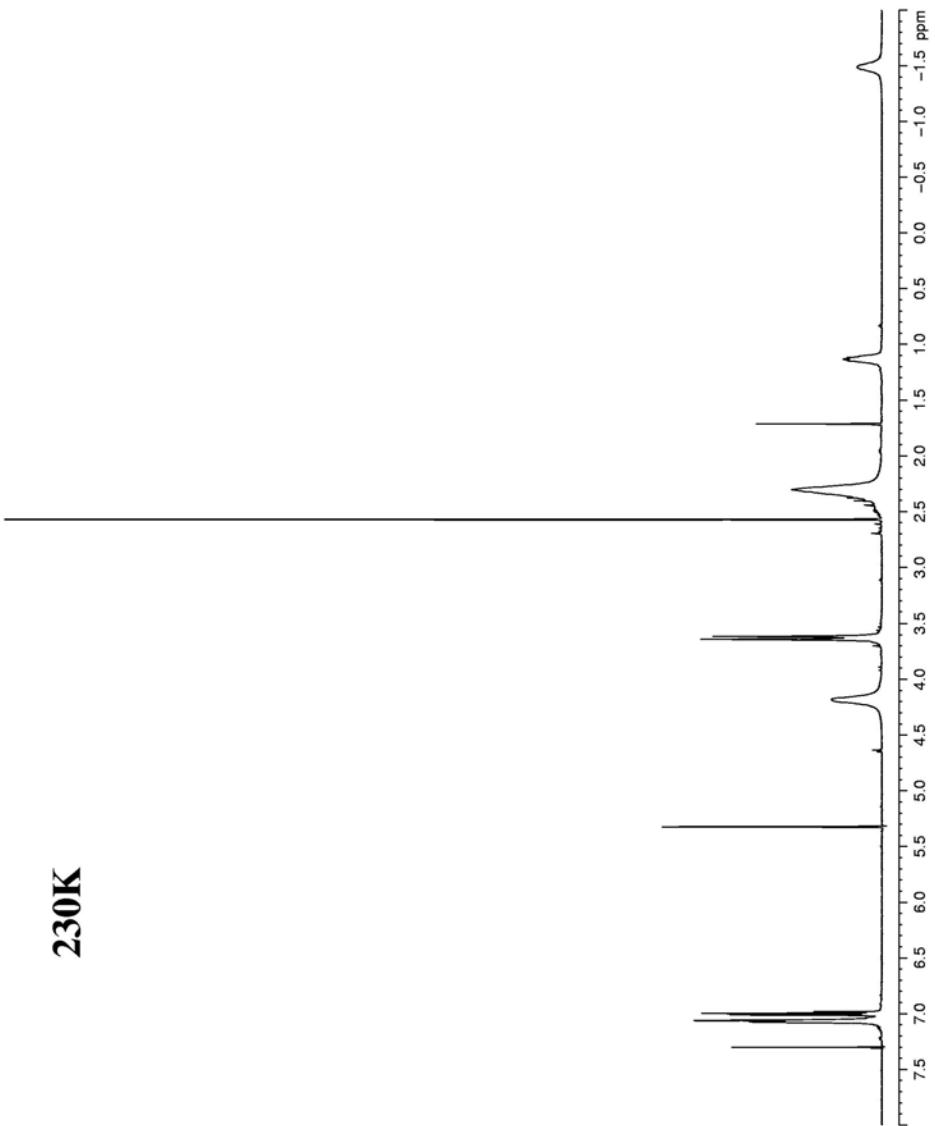
¹H NMR spectrum of **1** at 250K in 3:1 CD₂Cl₂:CDCl₃



¹H NMR spectrum of **1** at 240K in 3:1 CD₂Cl₂:CDCl₃

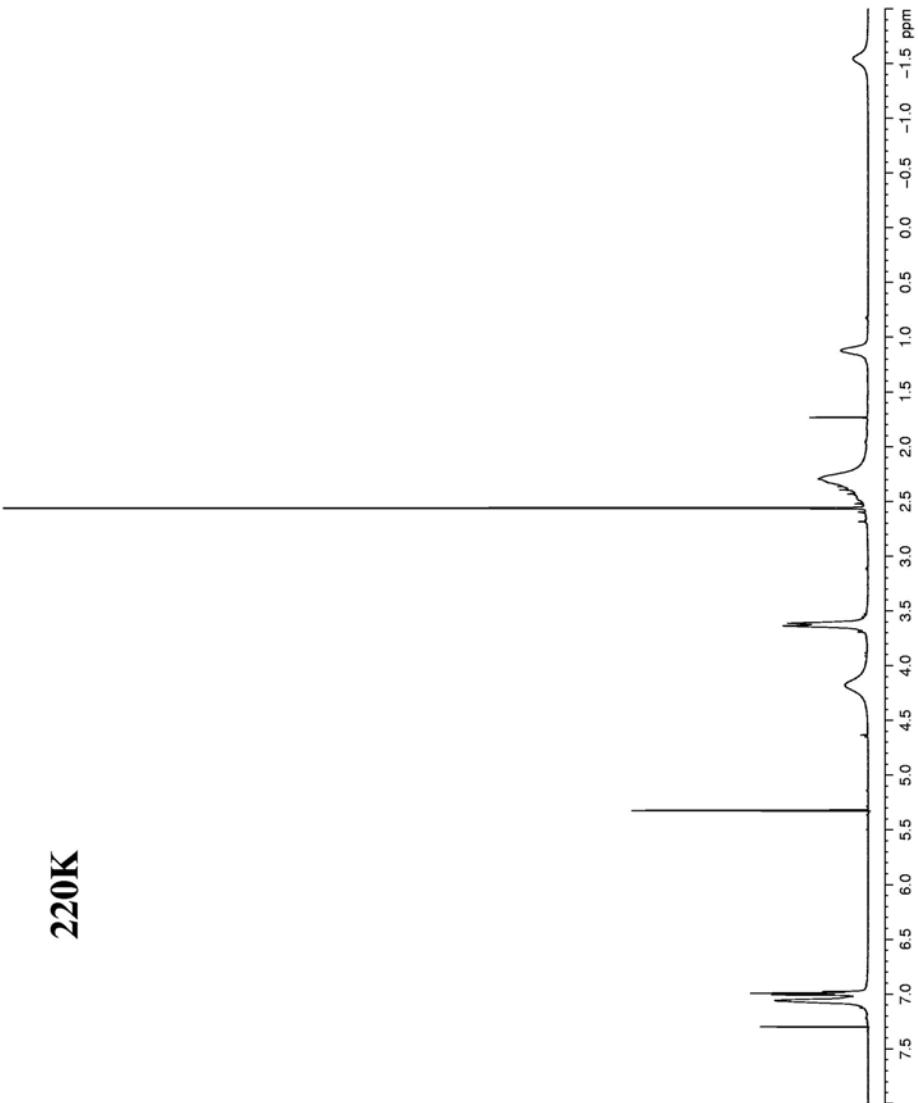


¹H NMR spectrum of **1** at 230K in 3:1 CD₂Cl₂:CDCl₃



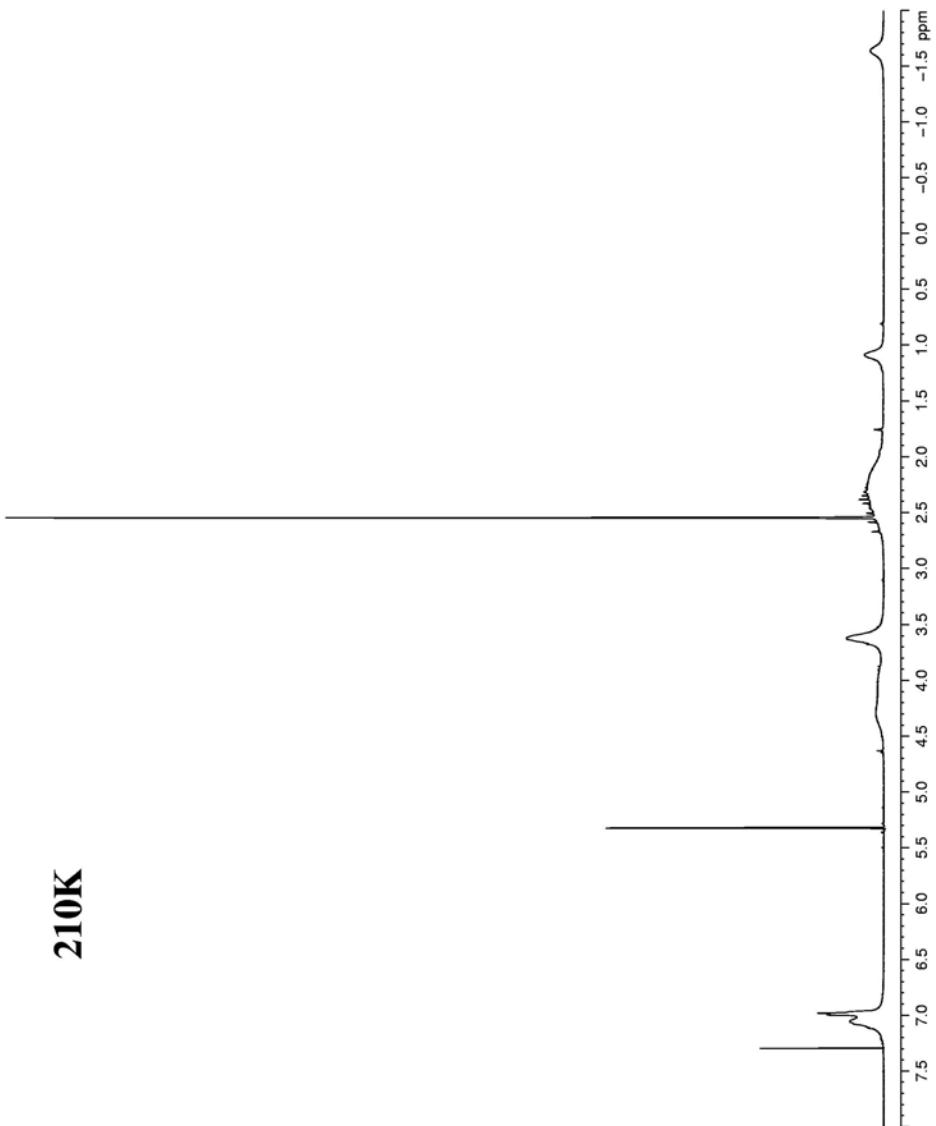
S(I)9

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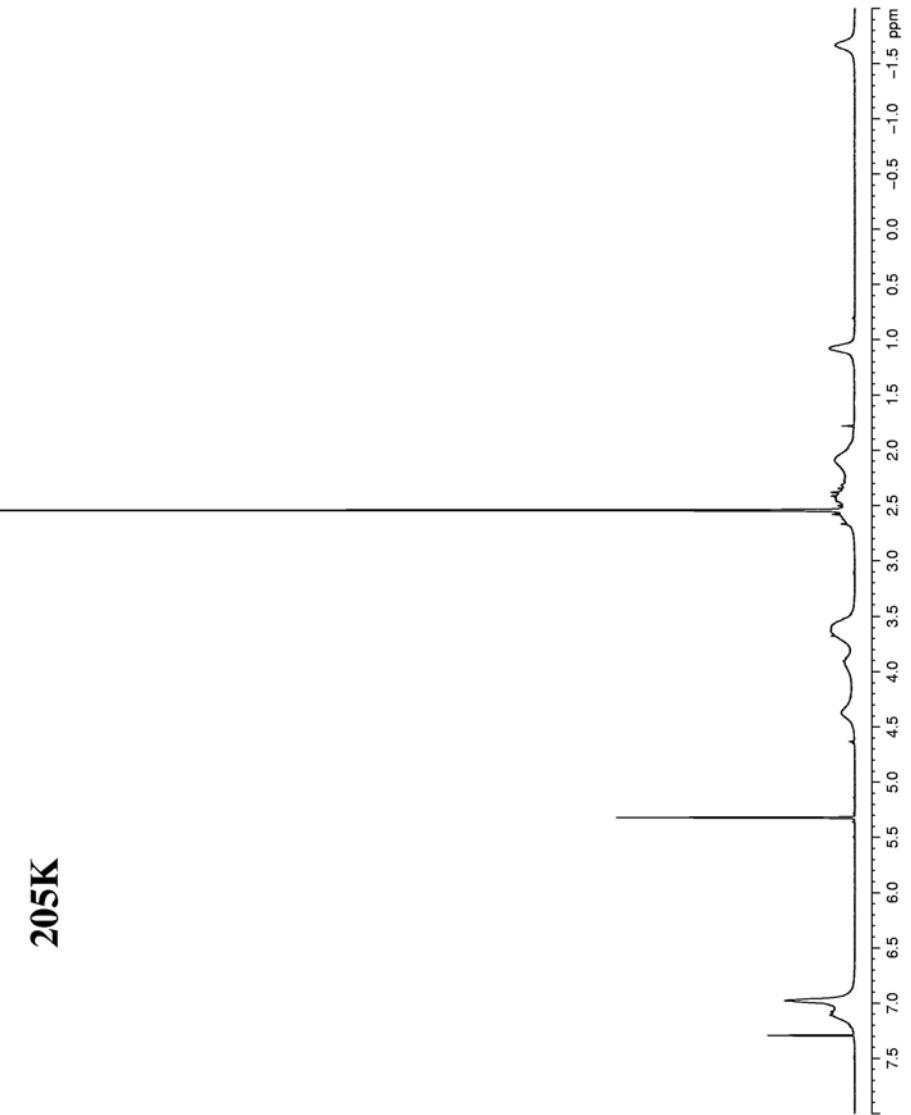


S(I)10

^1H NMR spectrum of **1** at 210K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$

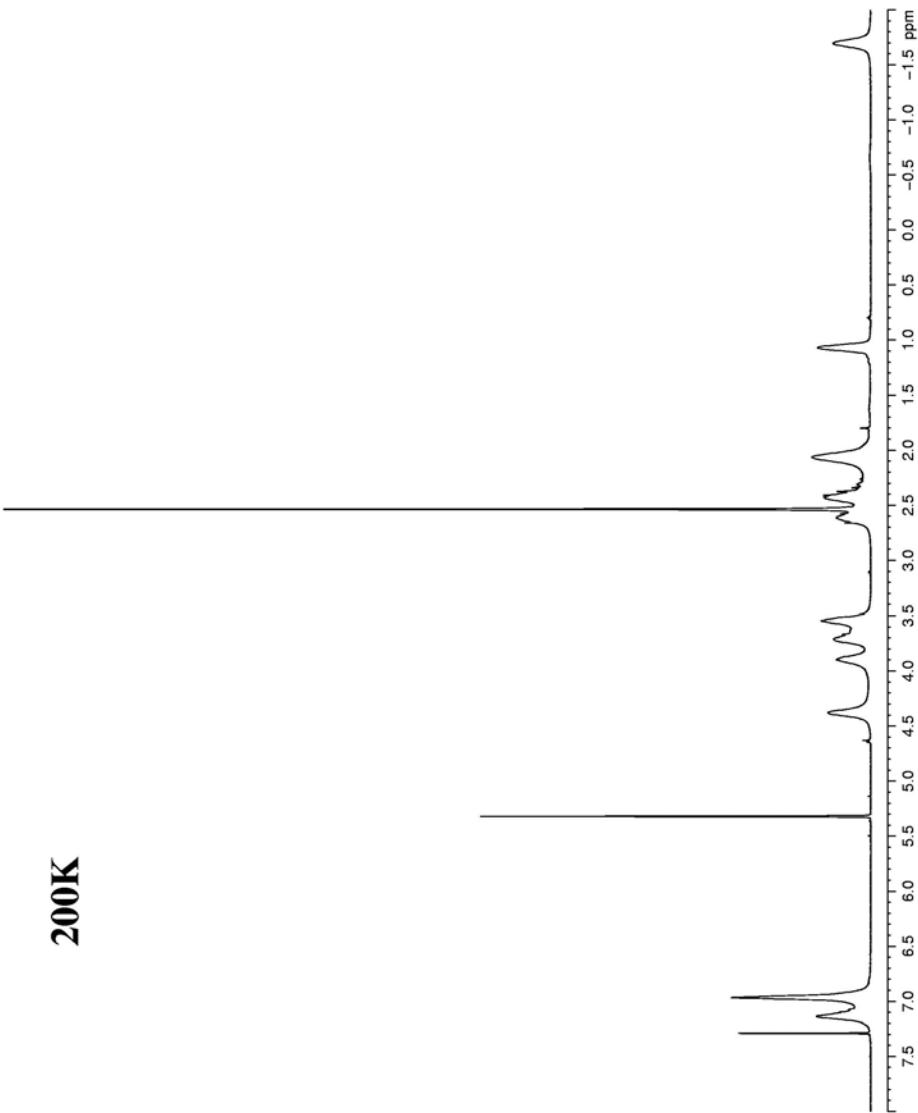


¹H NMR spectrum of **1** at 205K in 3:1 CD₂Cl₂:CDCl₃

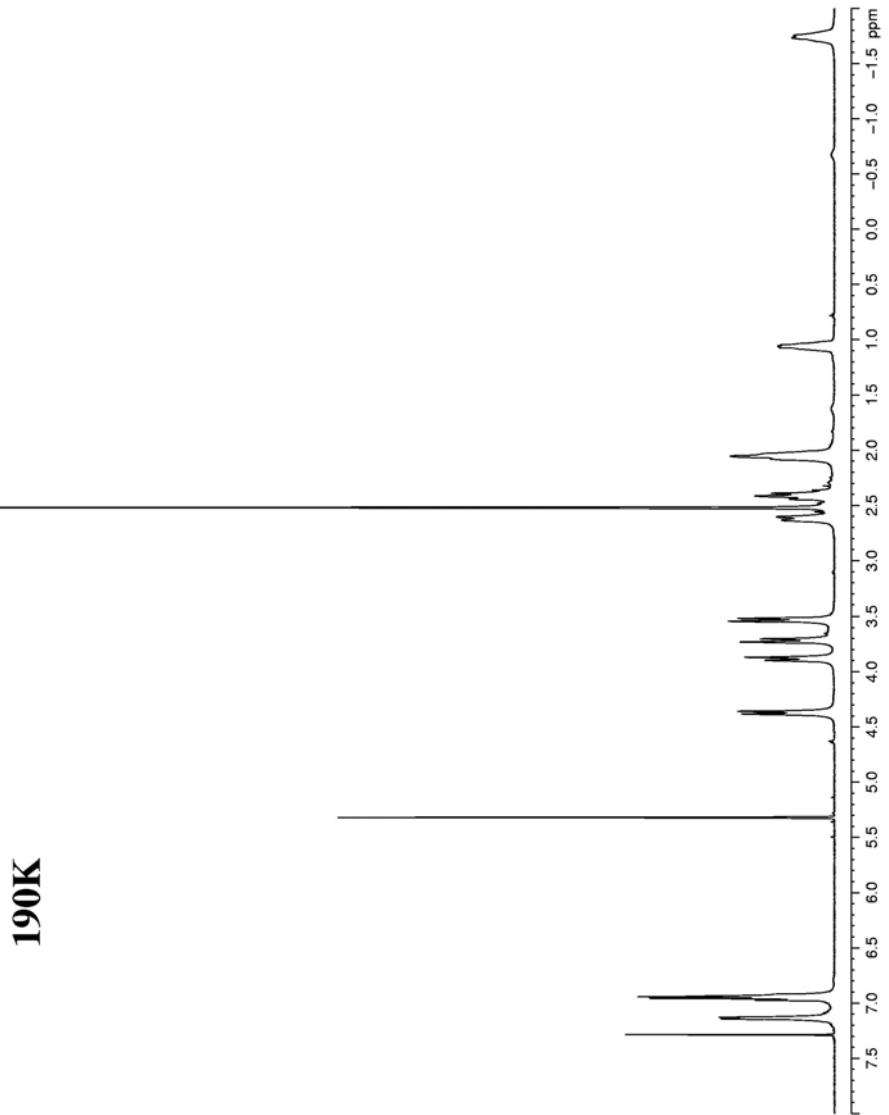


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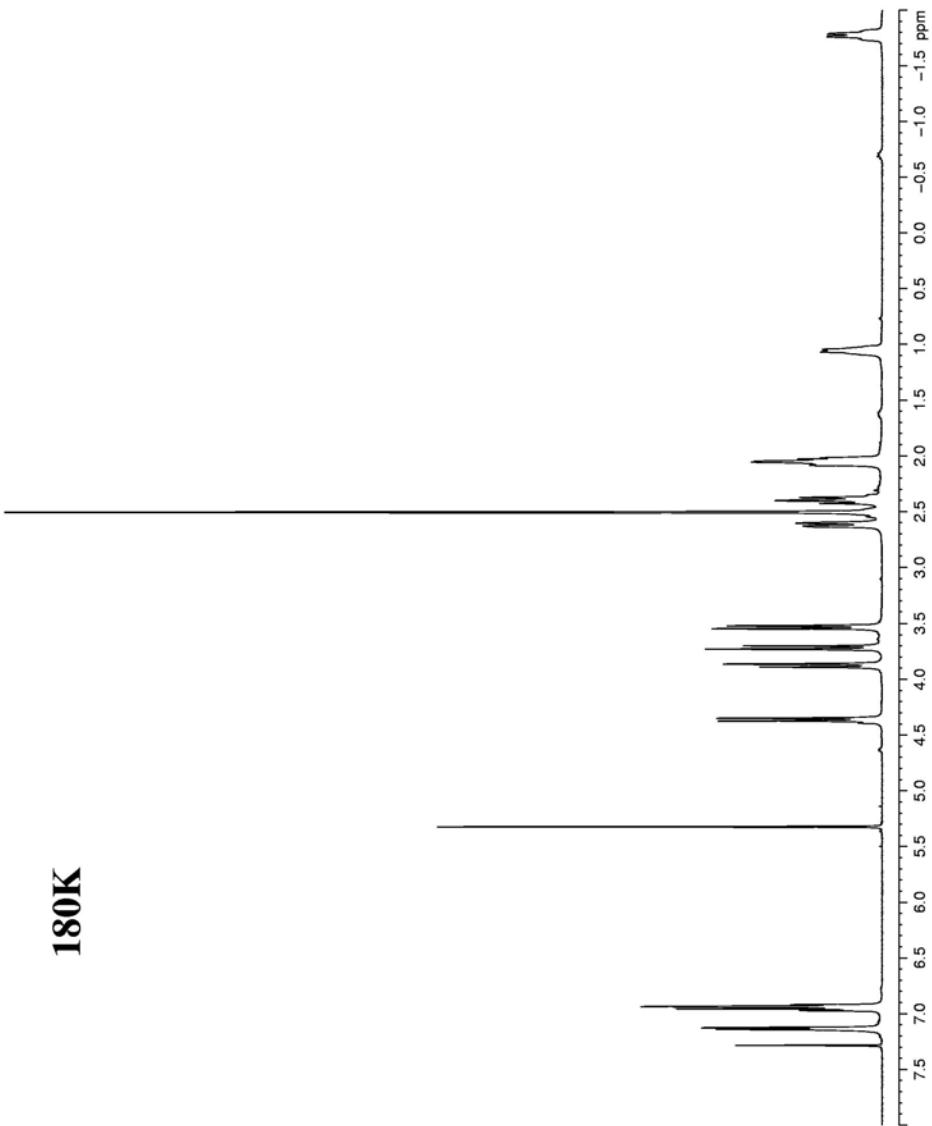
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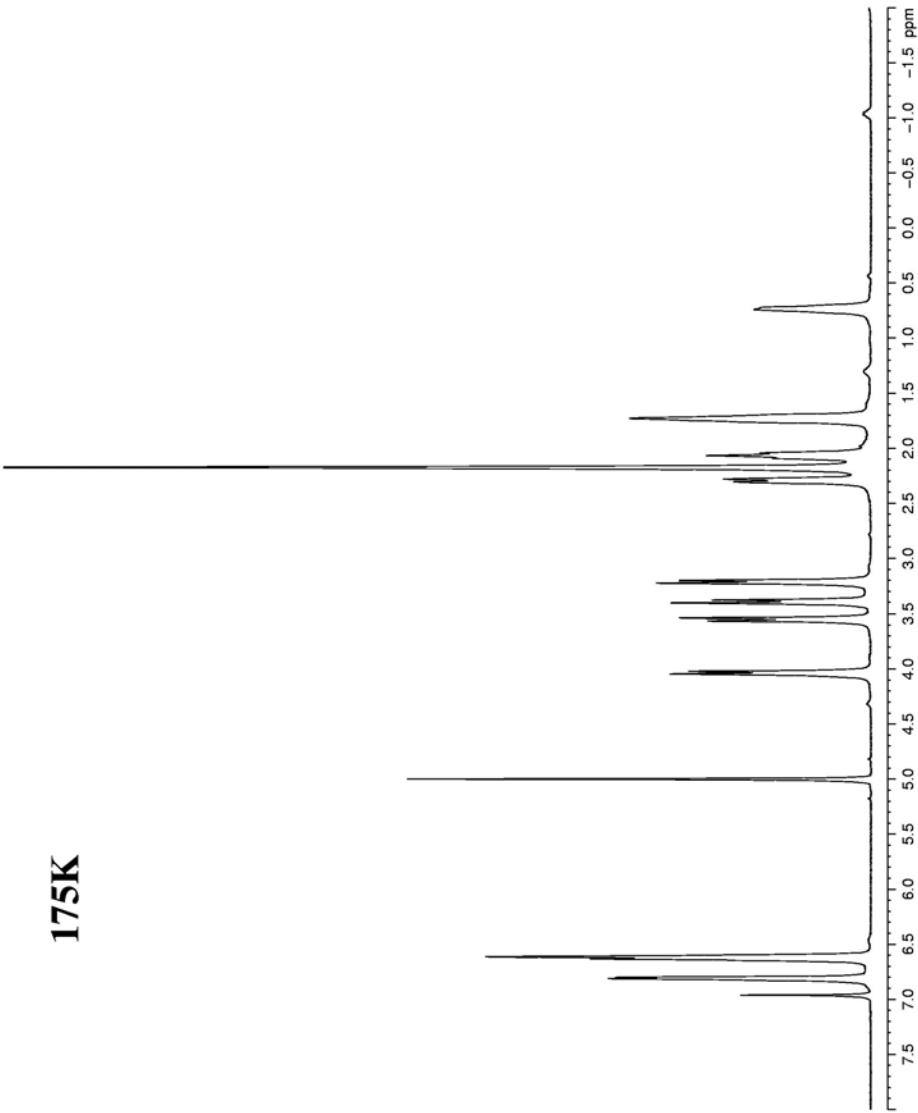
¹H NMR spectrum of **1** at 190K in 3:1 CD₂Cl₂:CDCl₃



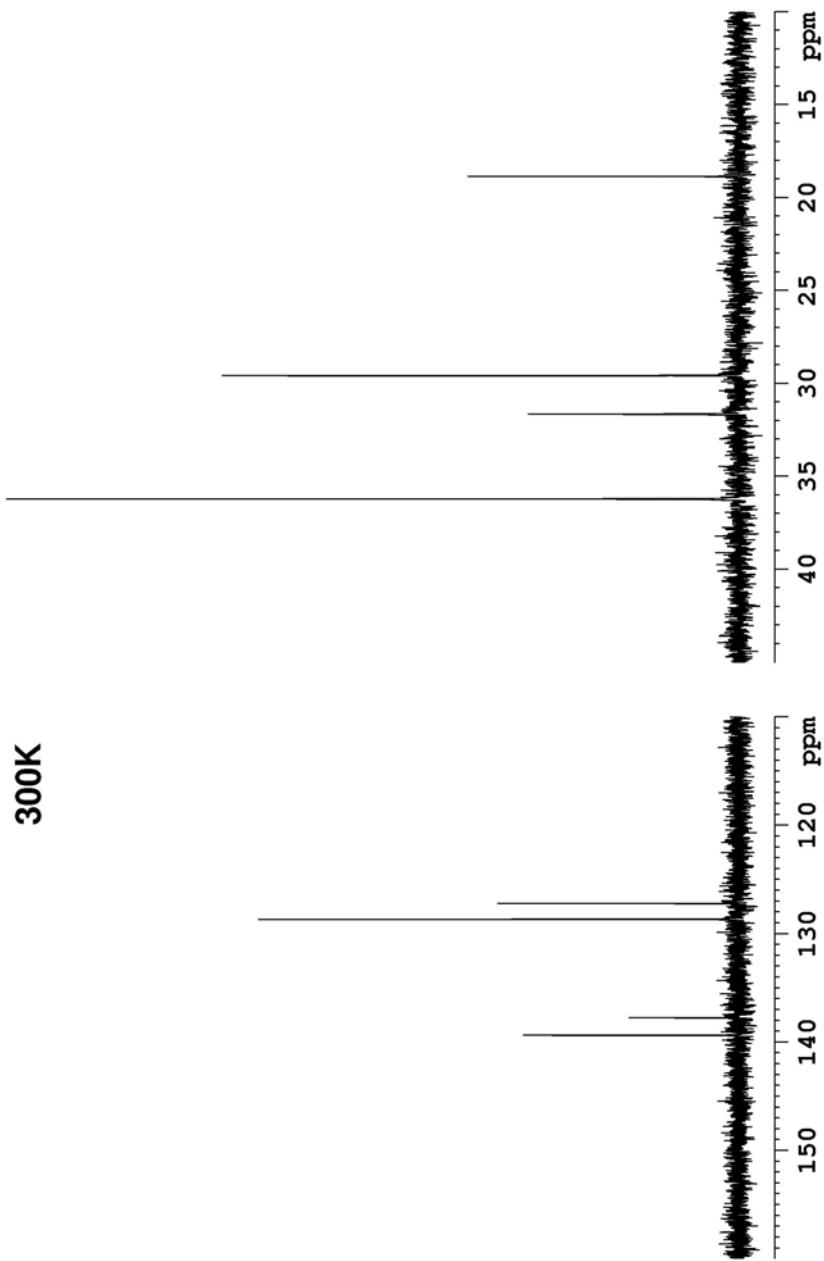
¹H NMR spectrum of **1** at 180K in 3:1 CD₂Cl₂:CDCl₃



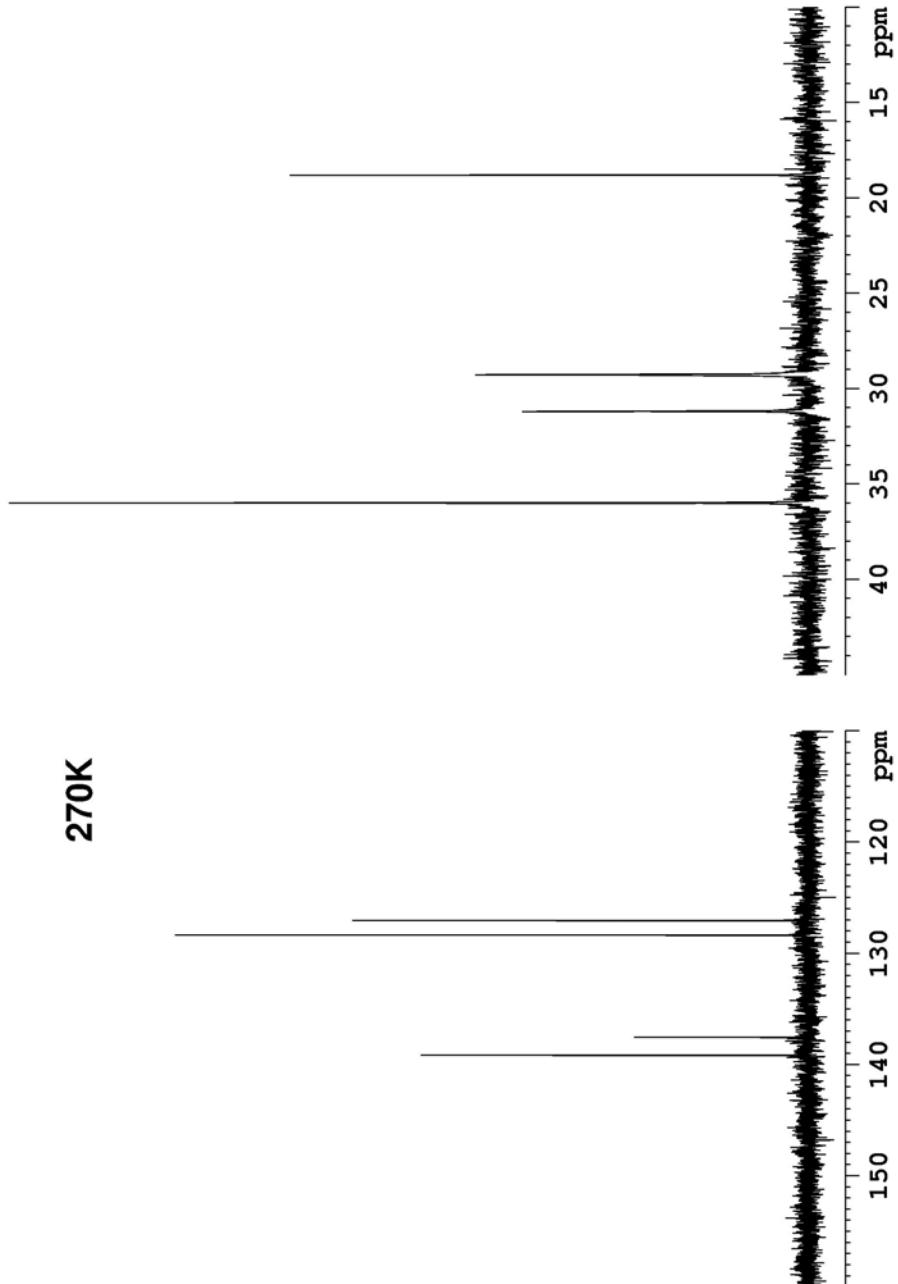
¹H NMR spectrum of **1** at 175K in 3:1 CD₂Cl₂:CDCl₃



^{13}C NMR spectrum of **1** at 300K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$

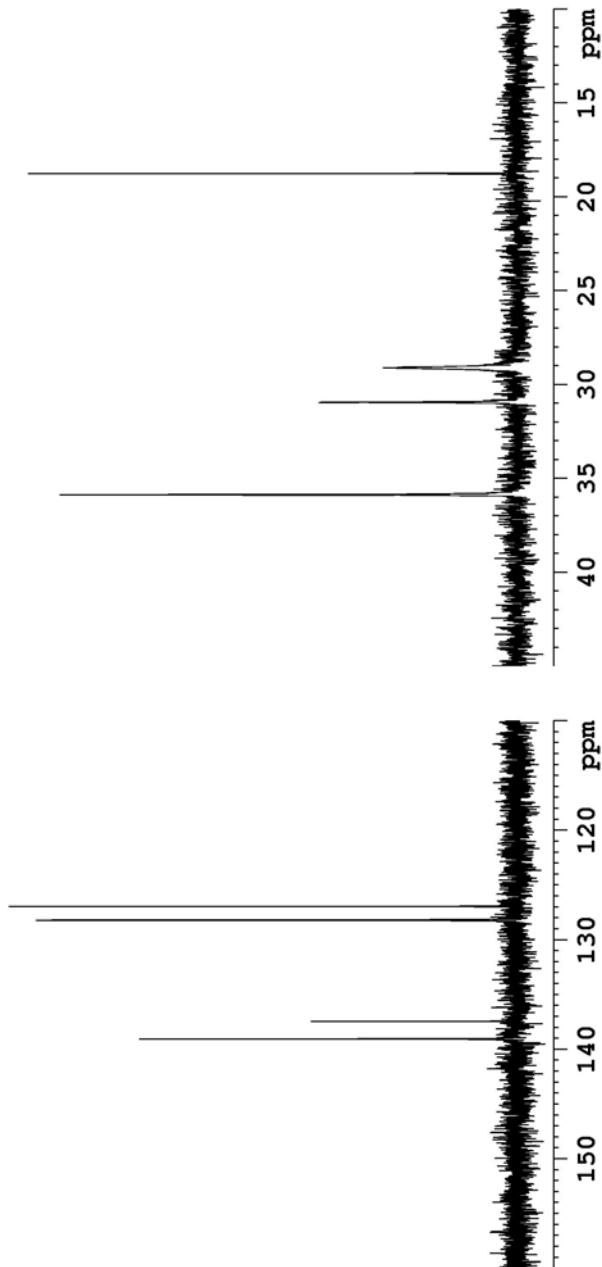


^{13}C NMR spectrum of **1** at 270K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$



^{13}C NMR spectrum of **1** at 250K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$

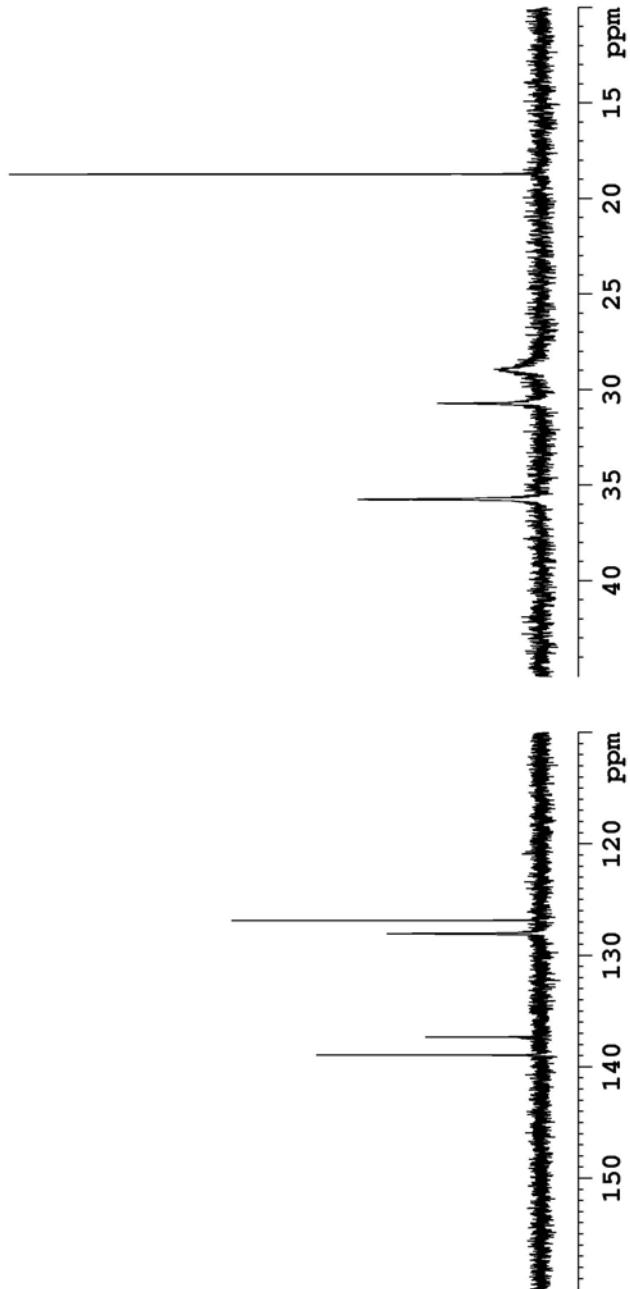
250K



S(I)19

^{13}C NMR spectrum of **1** at 240K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$

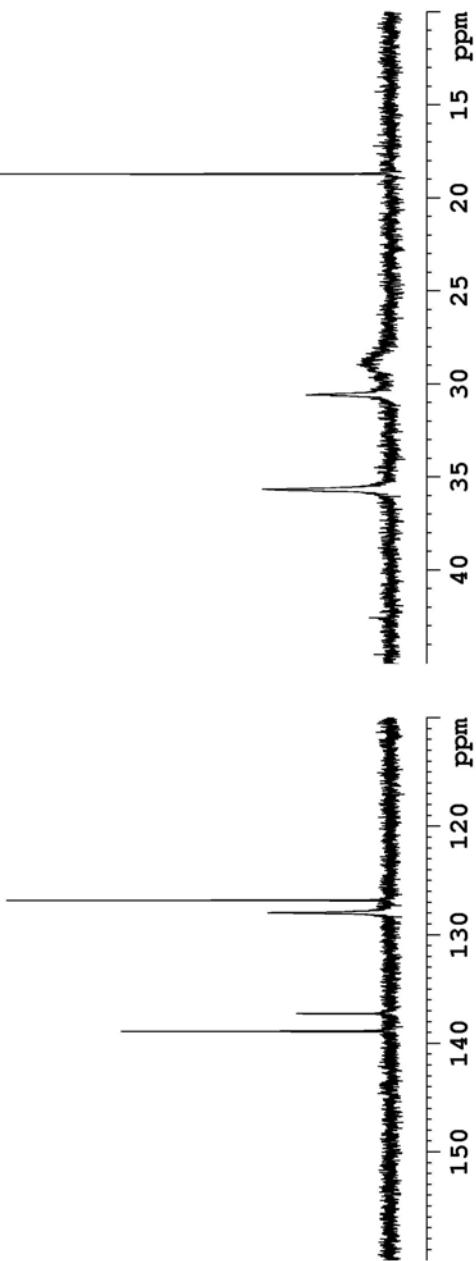
240K



S(I)20

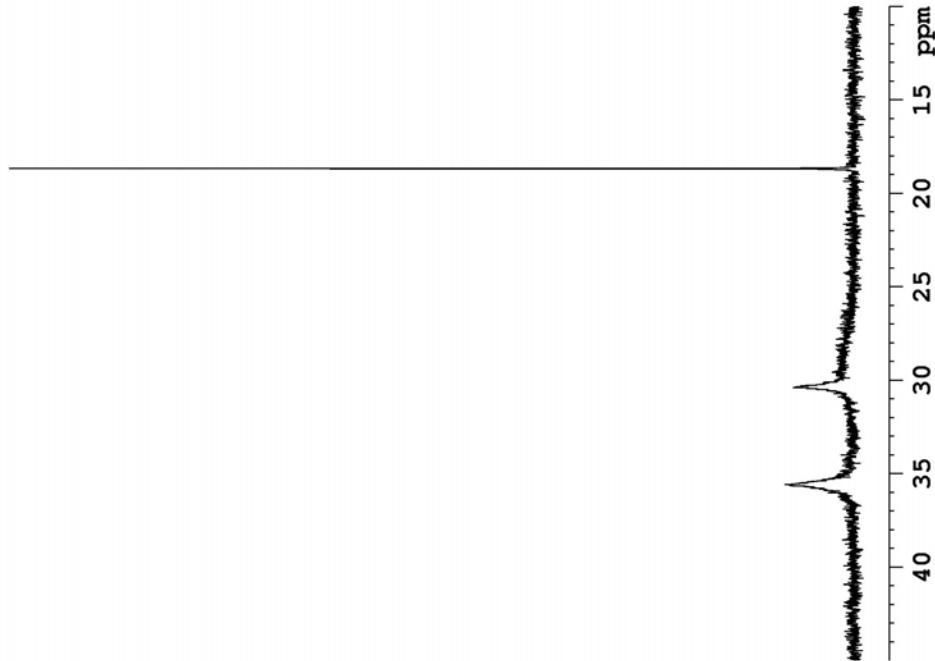
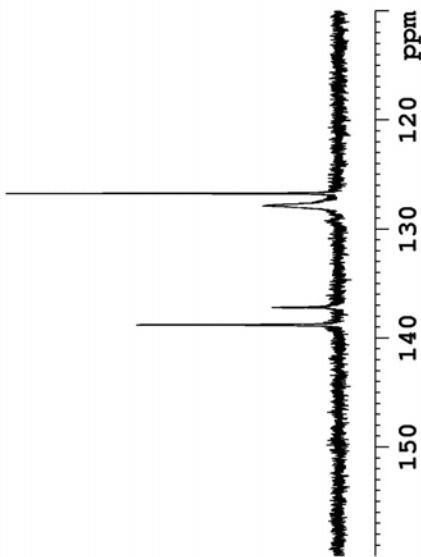
^{13}C NMR spectrum of **1** at 230K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$

230K

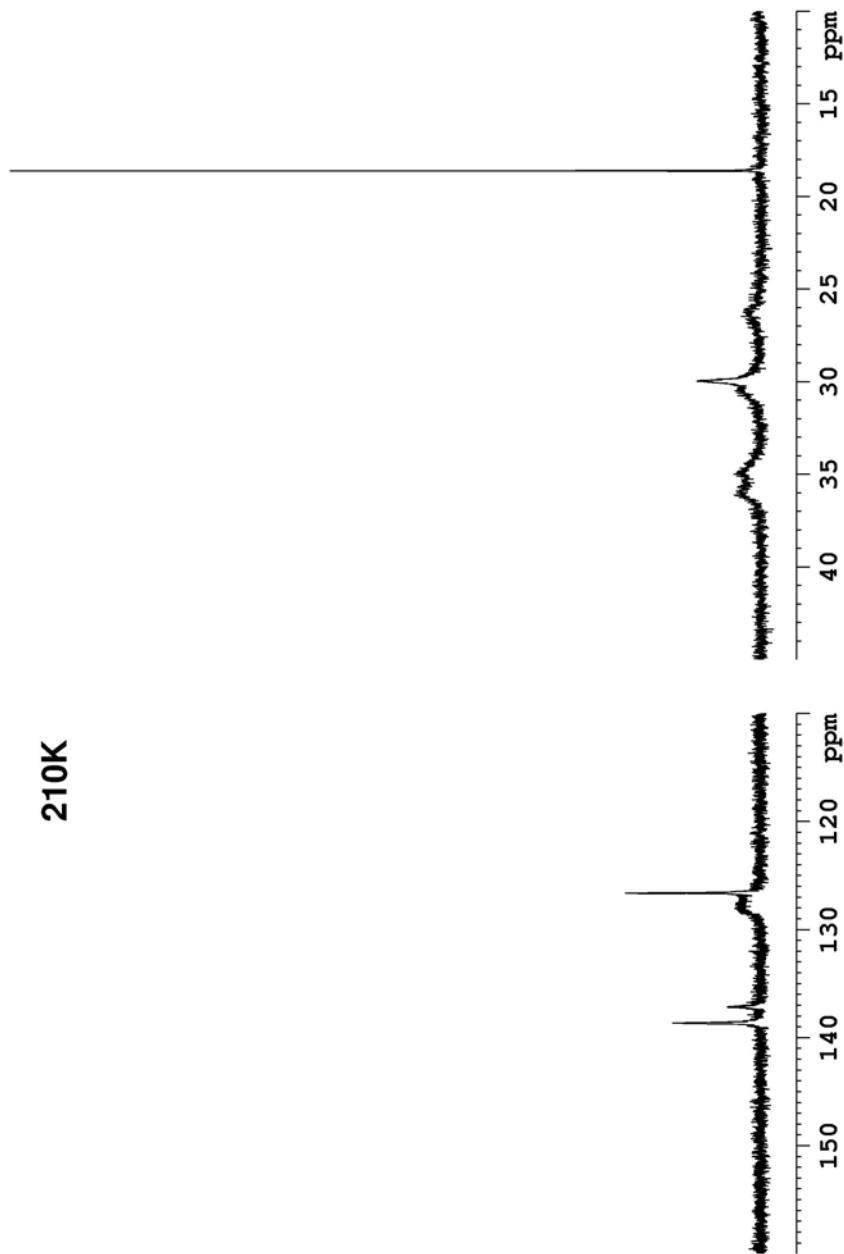


^{13}C NMR spectrum of **1** at 220K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$

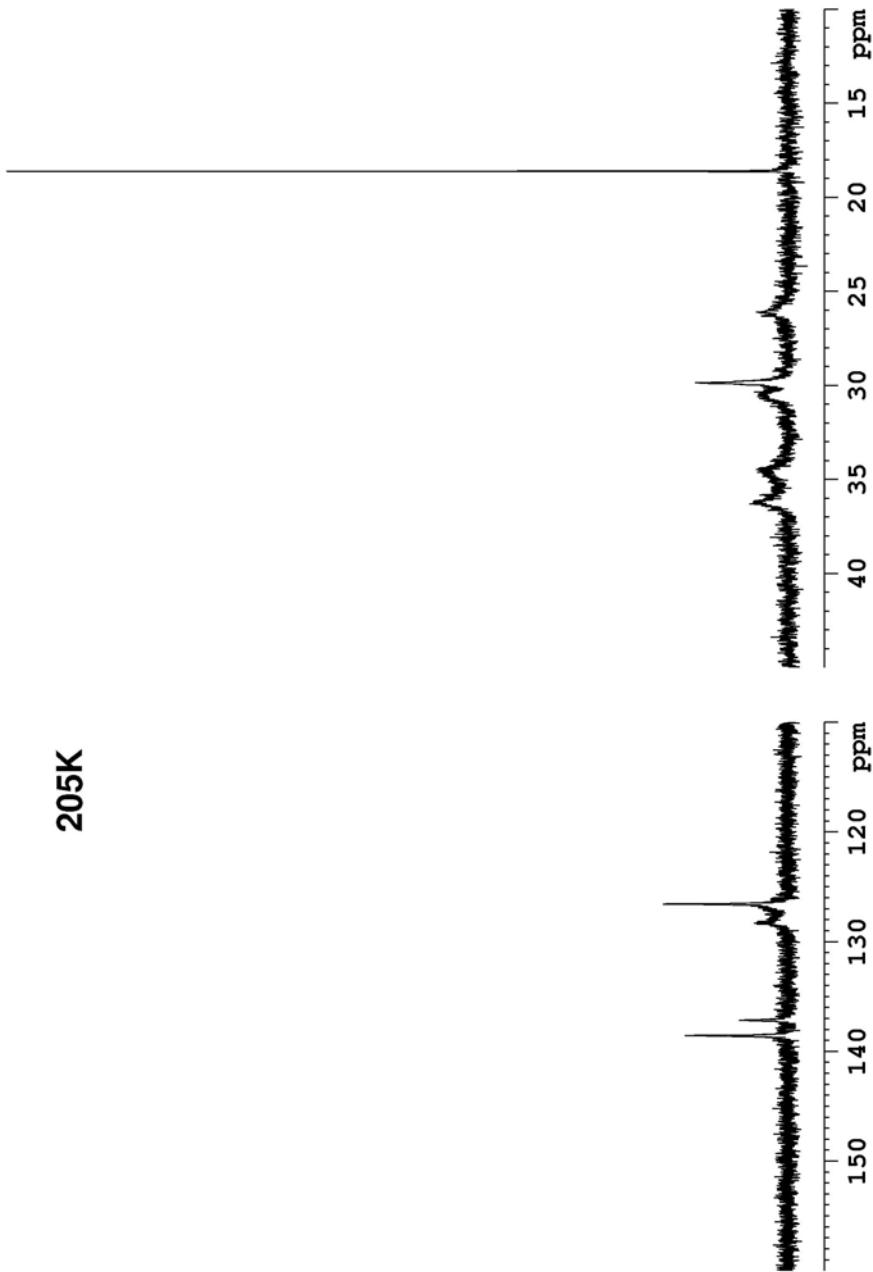
220K



^{13}C NMR spectrum of **1** at 210K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$

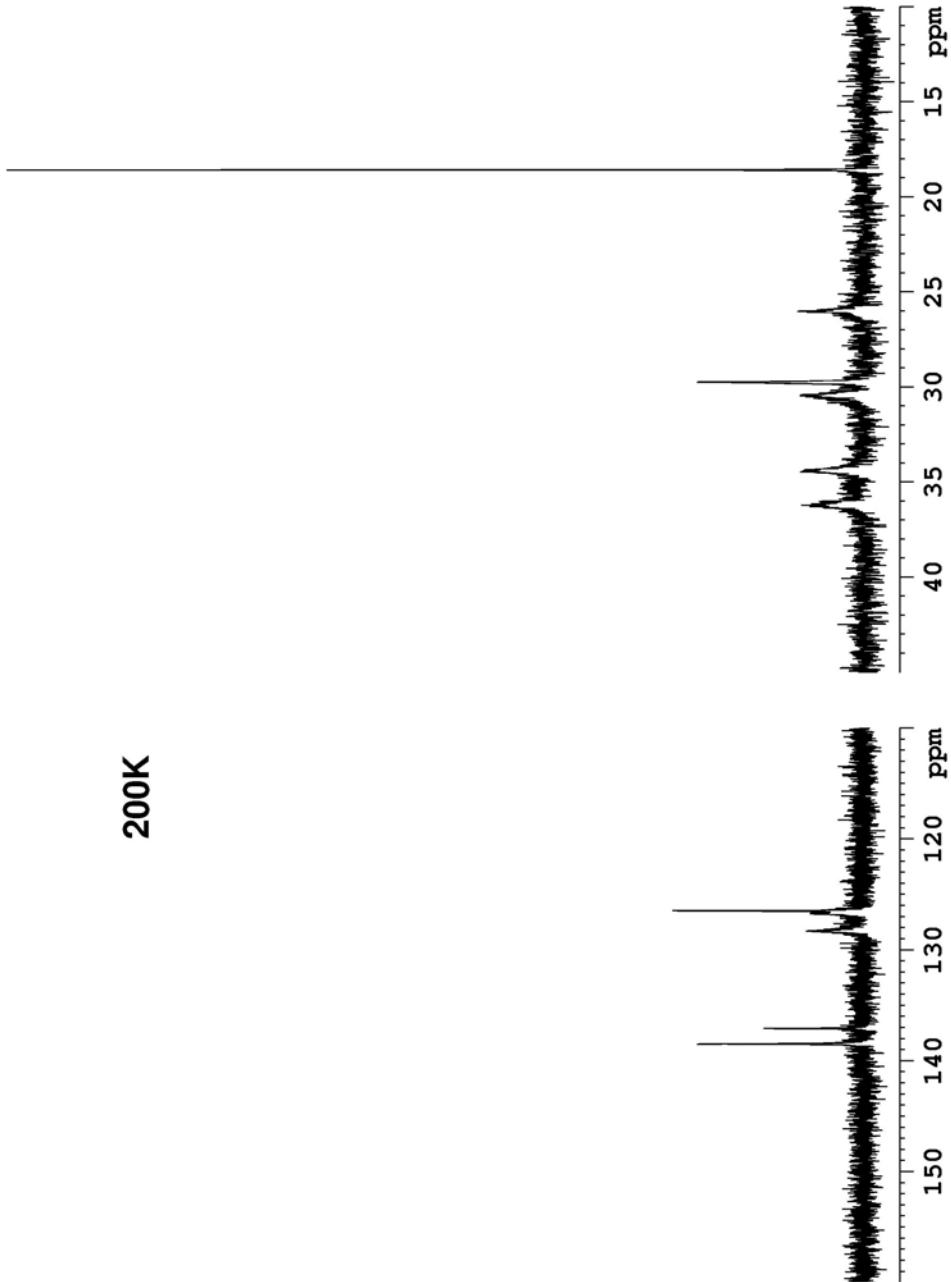


^{13}C NMR spectrum of **1** at 205K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$



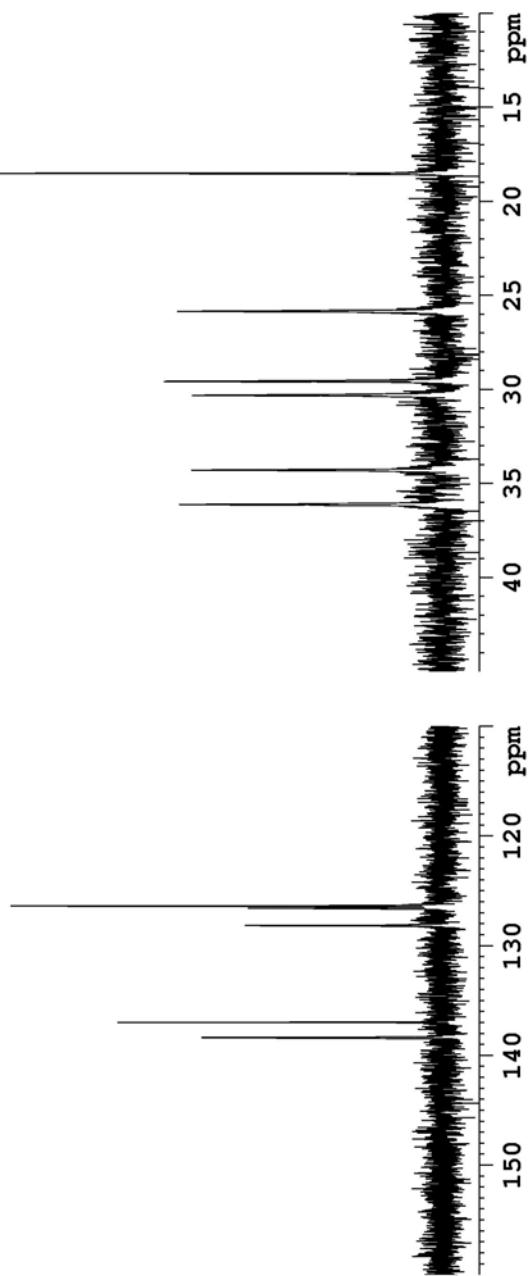
205K

^{13}C NMR spectrum of **1** at 200K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$



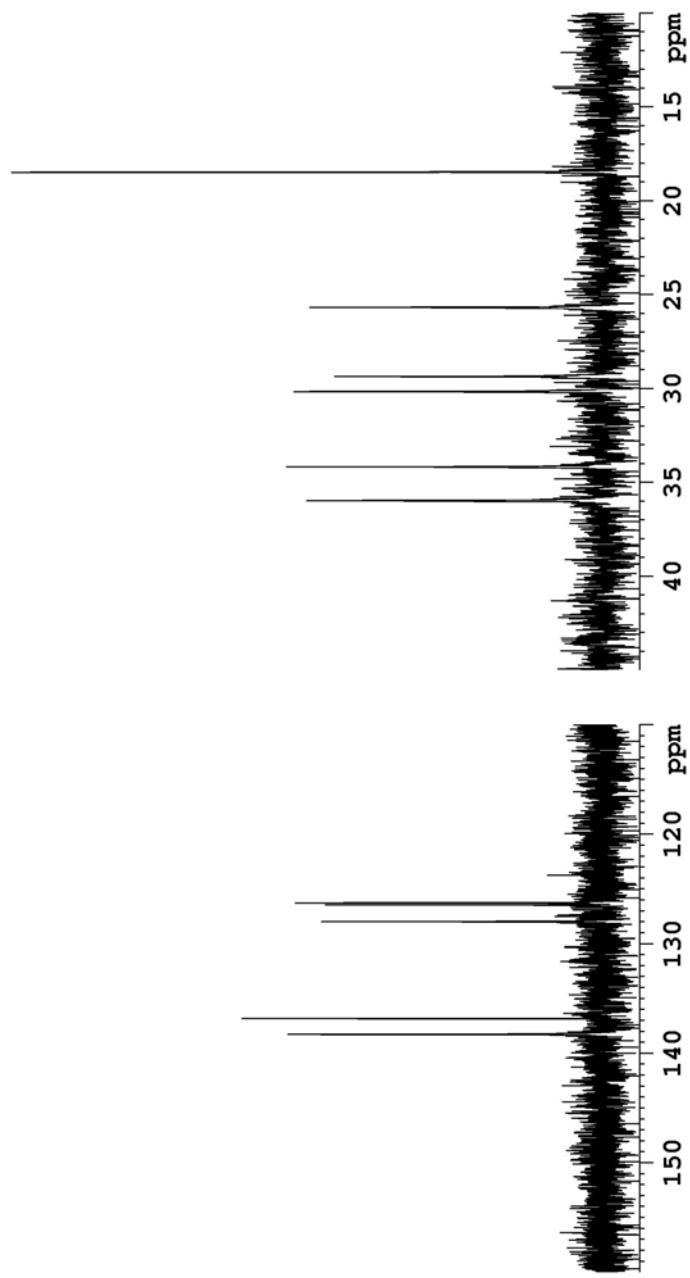
^{13}C NMR spectrum of **1** at 190K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$

190K

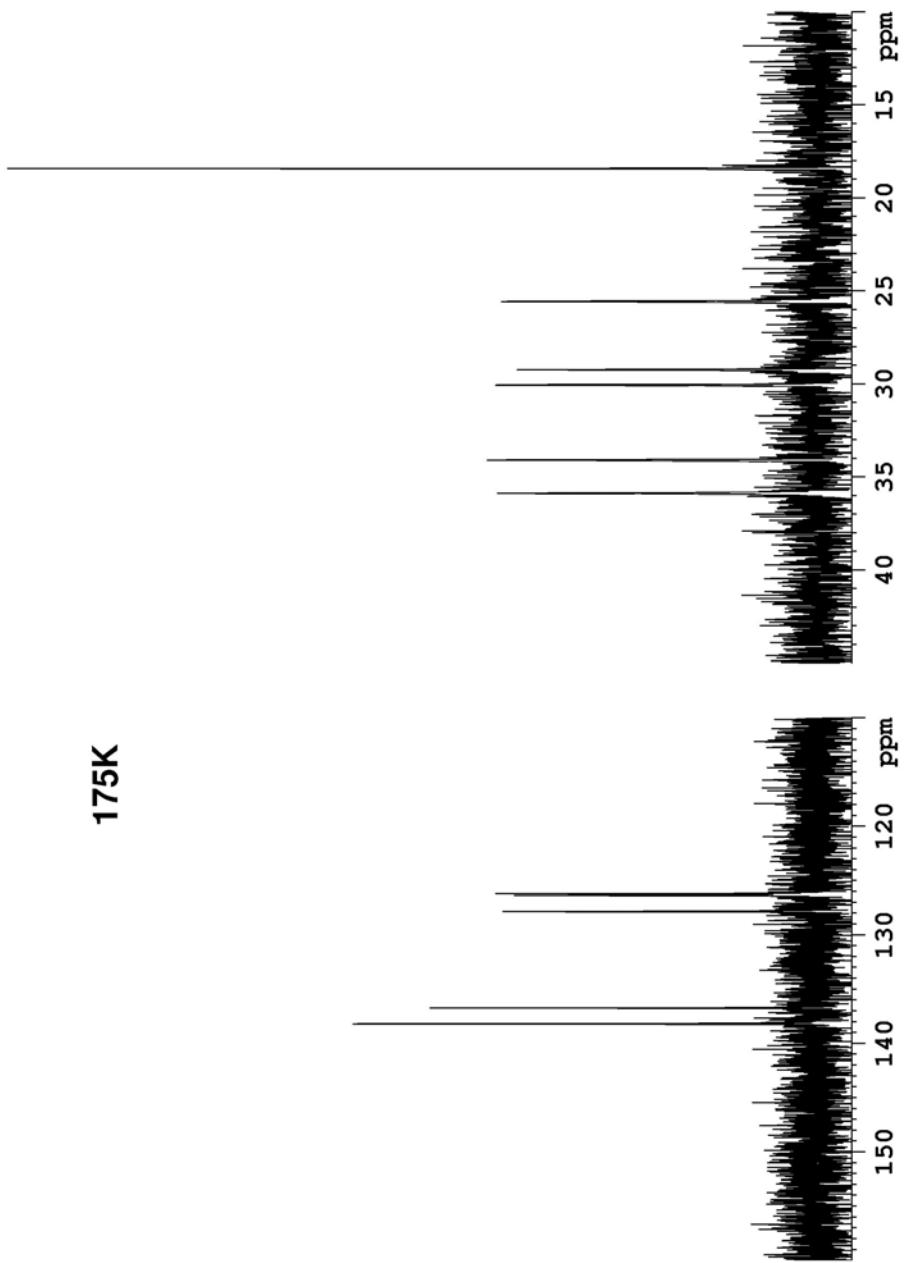


^{13}C NMR spectrum of **1** at 180K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$

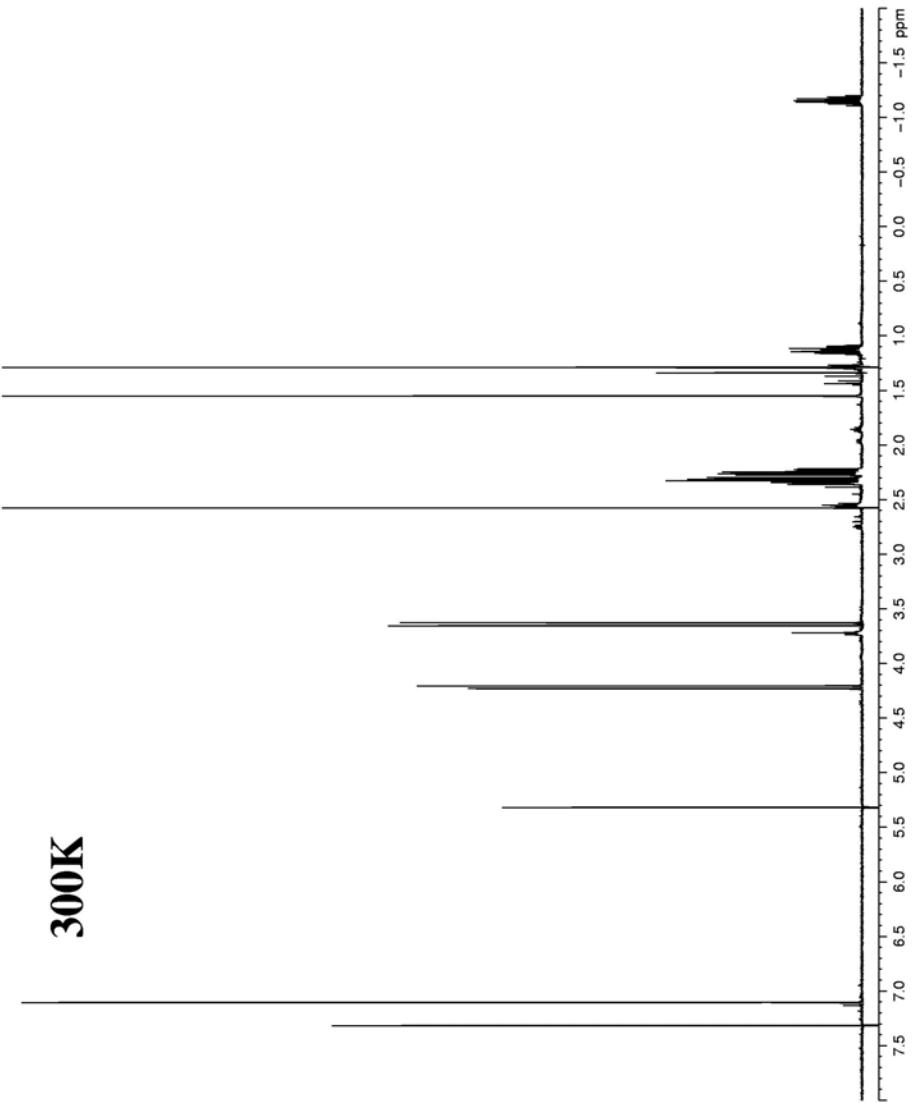
180K



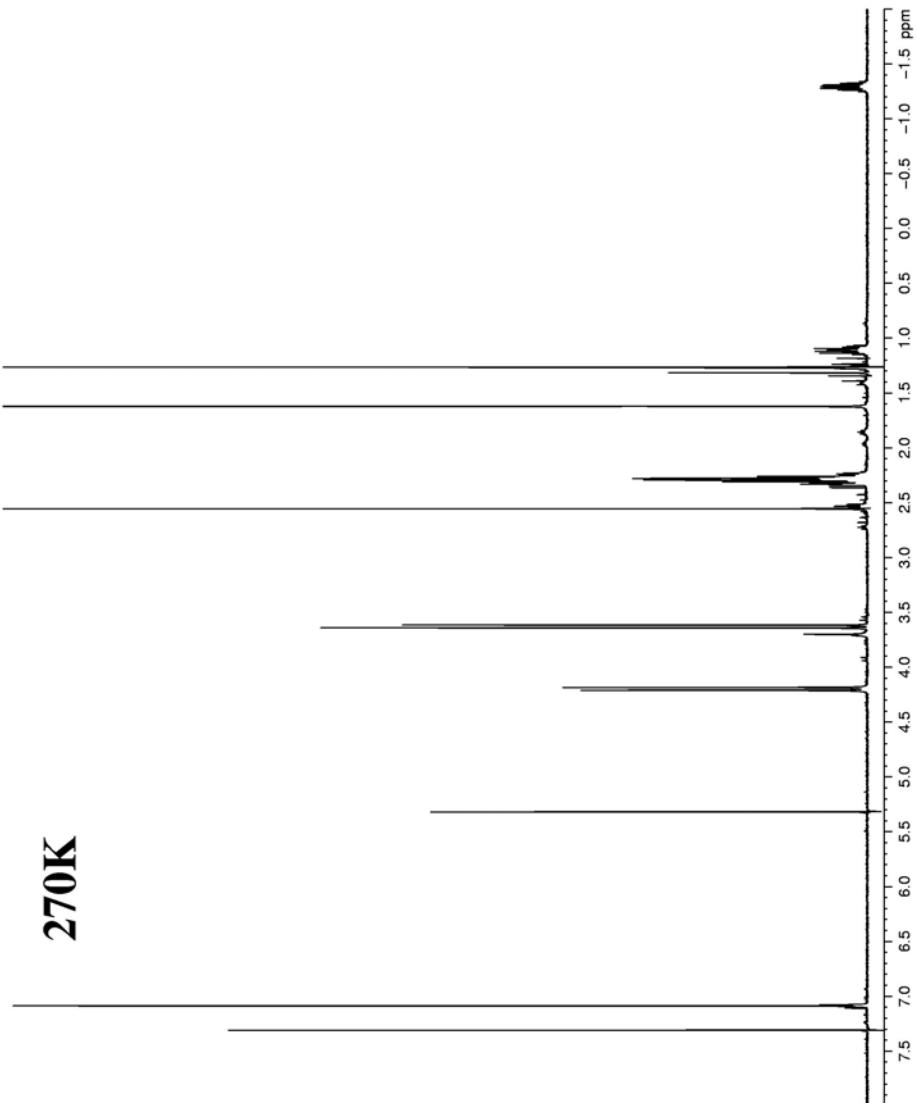
^{13}C NMR spectrum of **1** at 175K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$



¹H NMR spectrum of **2** at 300K in 3:1 CD₂Cl₂:CDCl₃

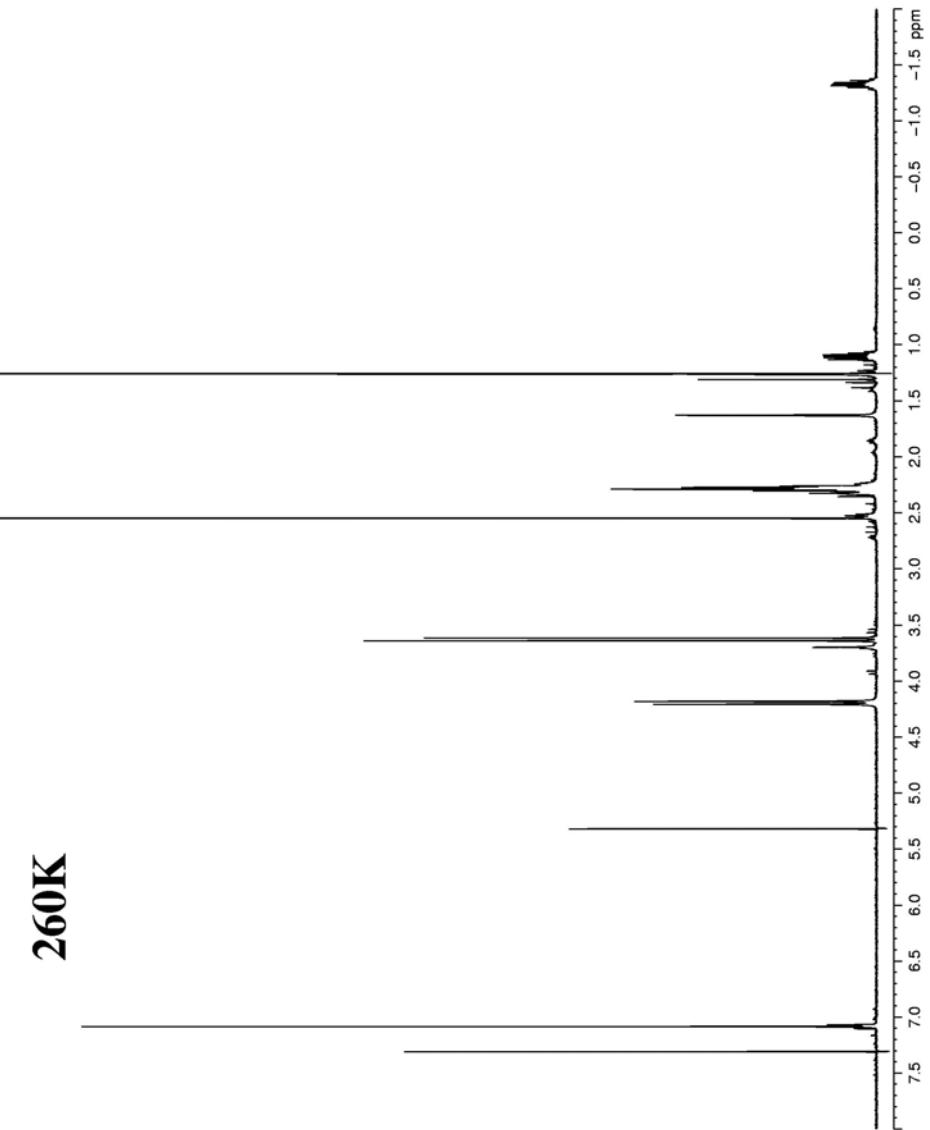


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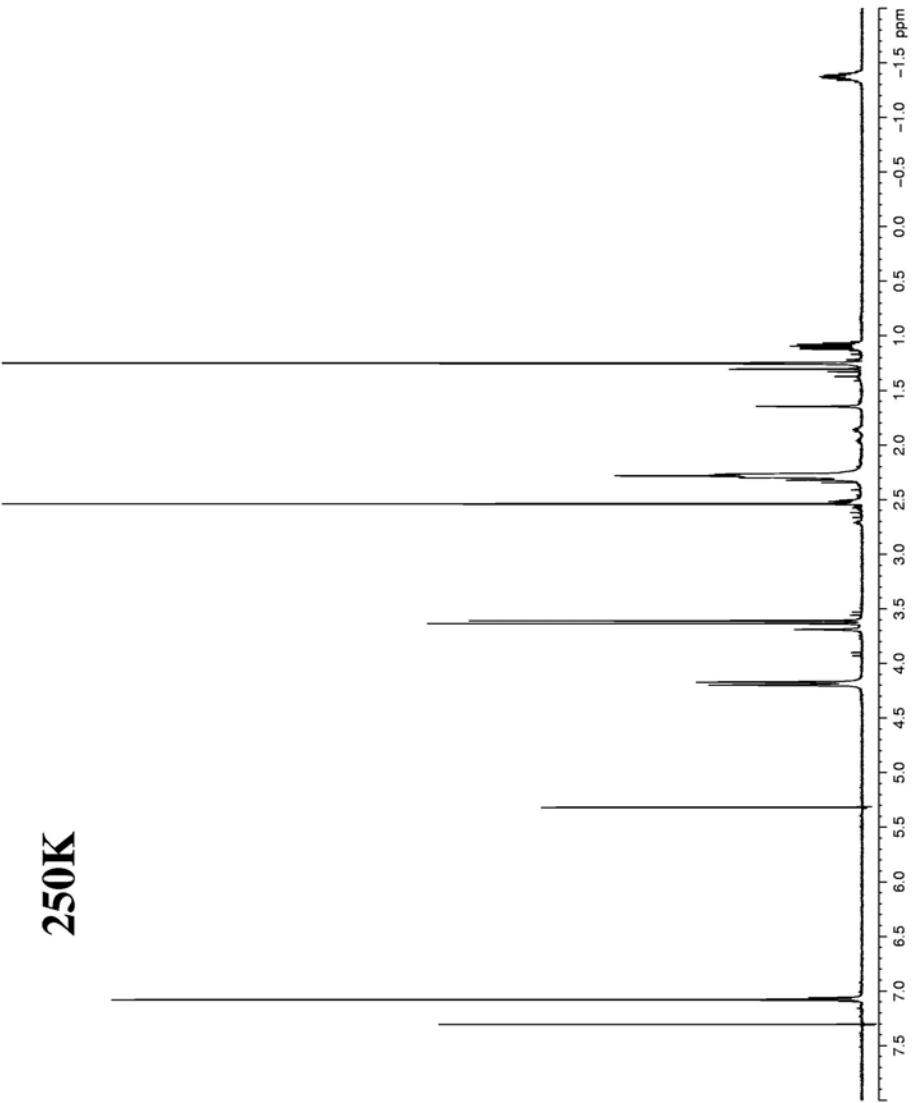
S(I)30

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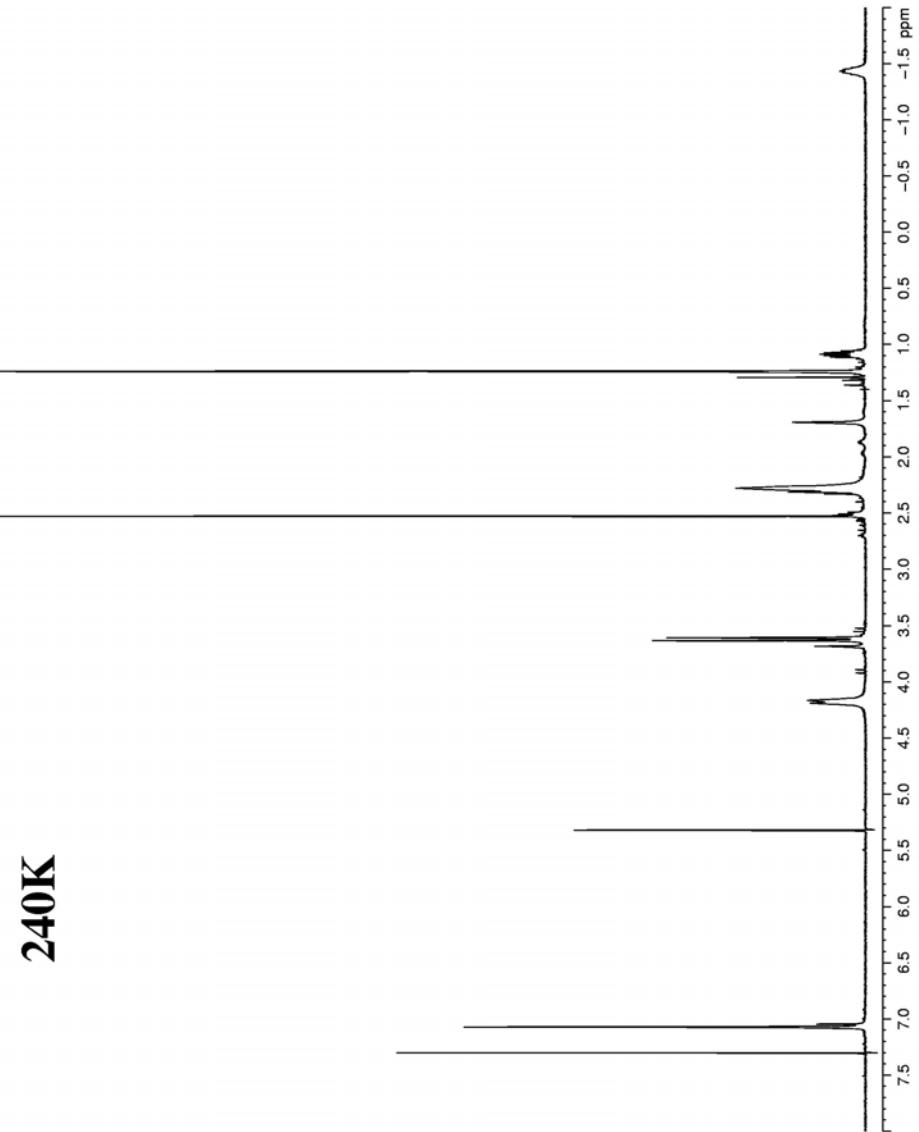


S(I)31

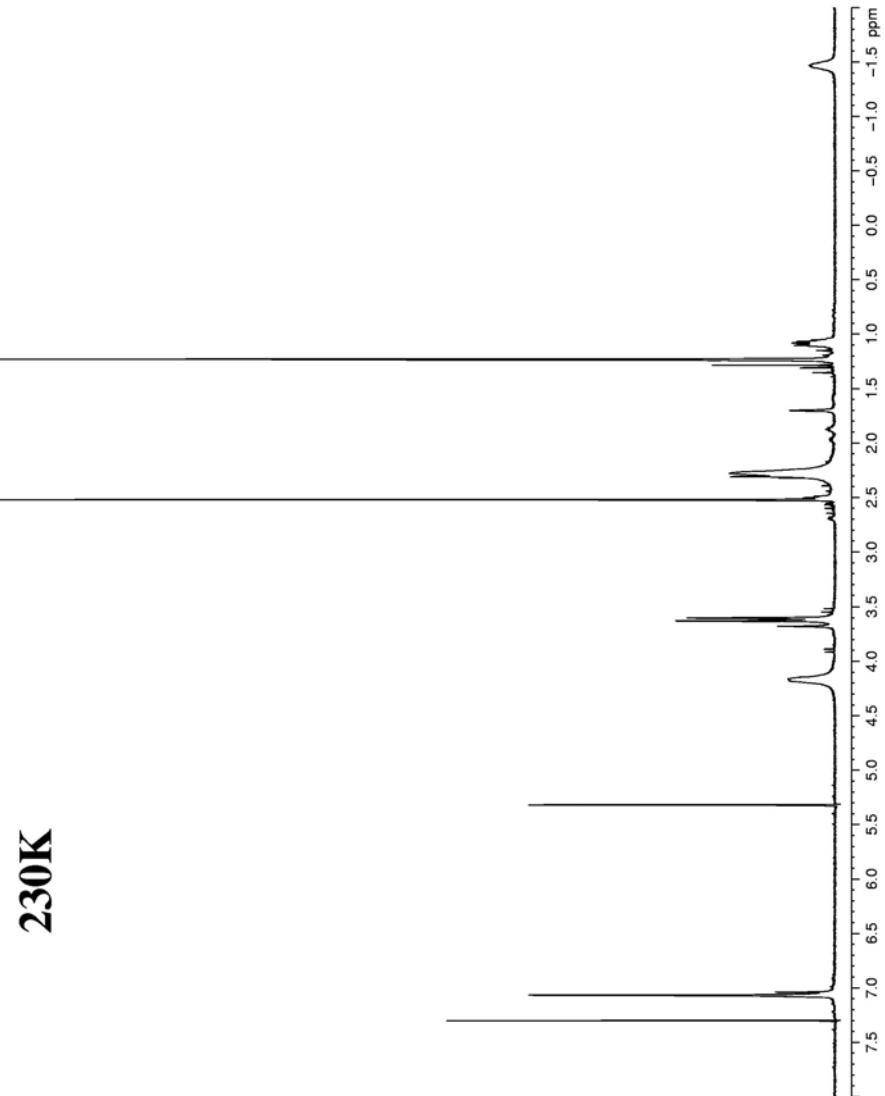
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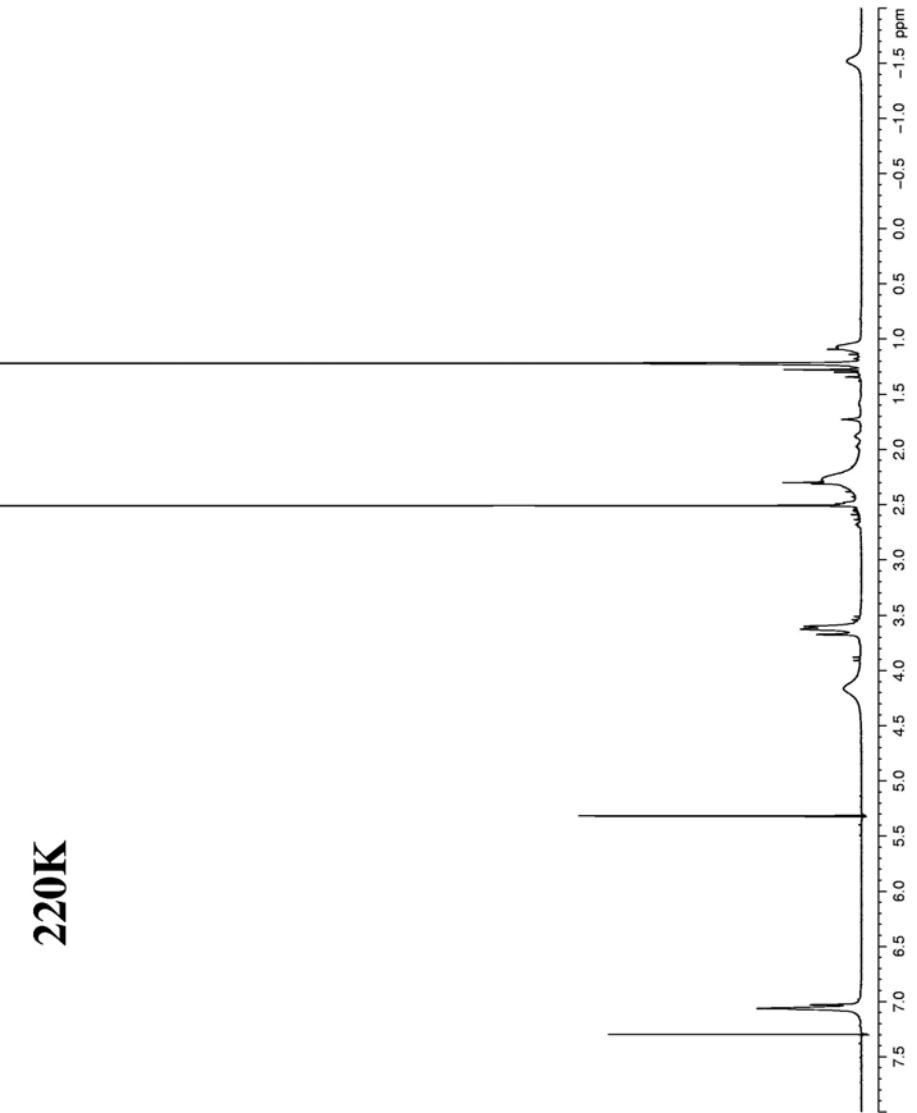
¹H NMR spectrum of **2** at 240K in 3:1 CD₂Cl₂:CDCl₃



¹H NMR spectrum of **2** at 230K in 3:1 CD₂Cl₂:CDCl₃

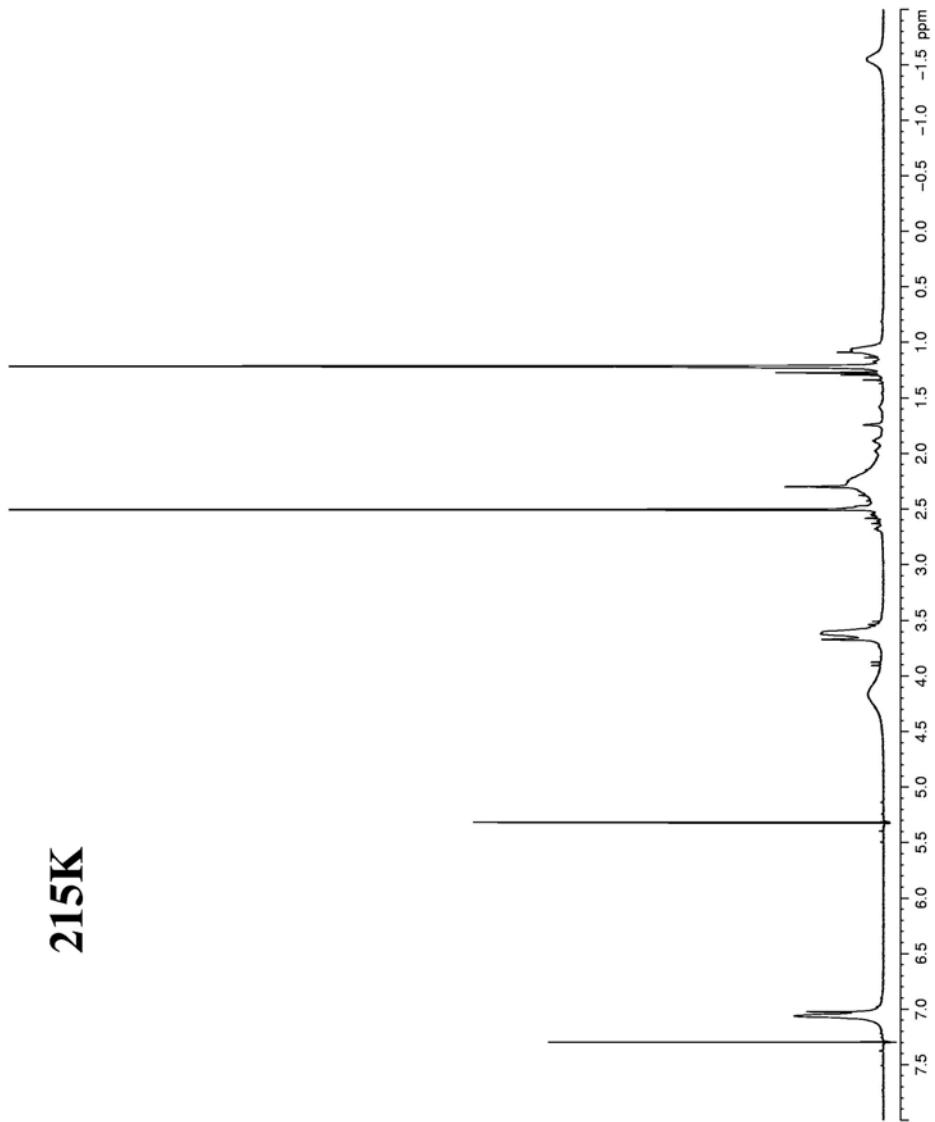


¹H NMR spectrum of **2** at 220K in 3:1 CD₂Cl₂:CDCl₃

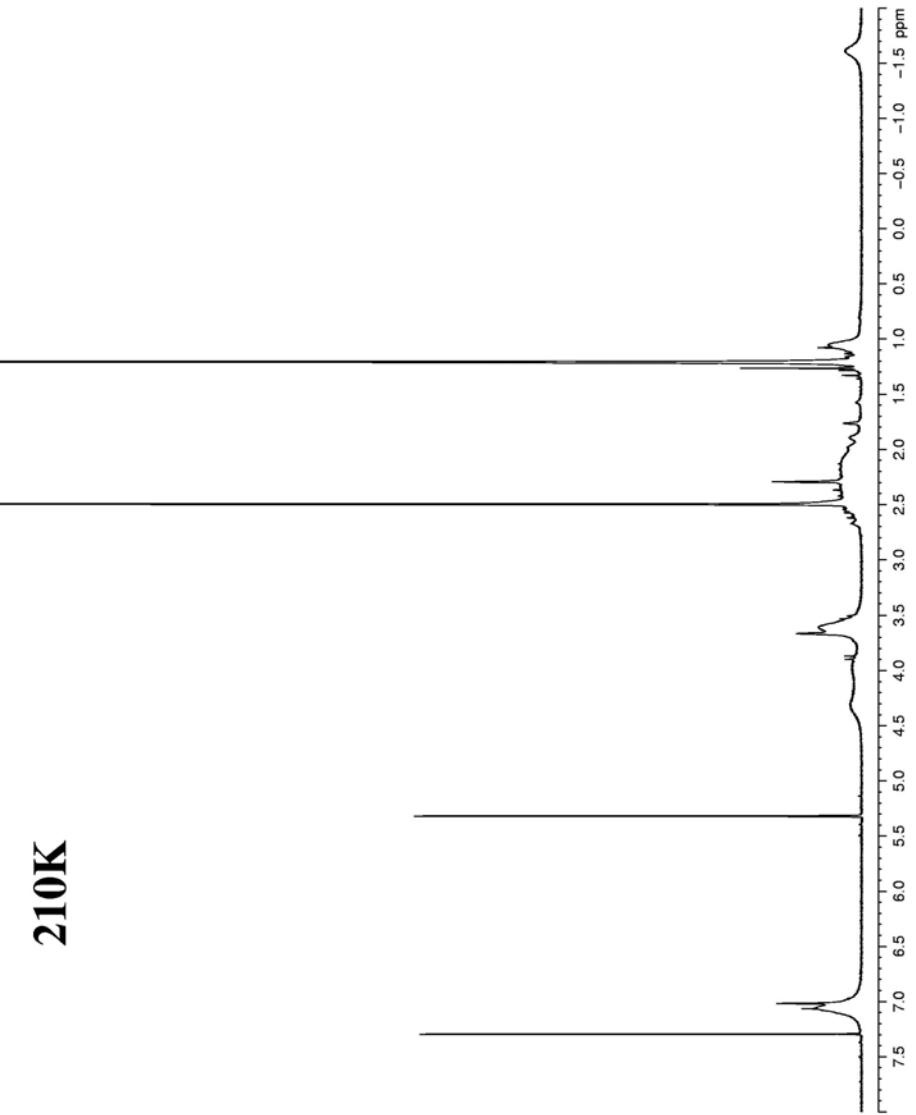


¹H NMR spectrum of **2** at 215K in 3:1 CD₂Cl₂:CDCl₃

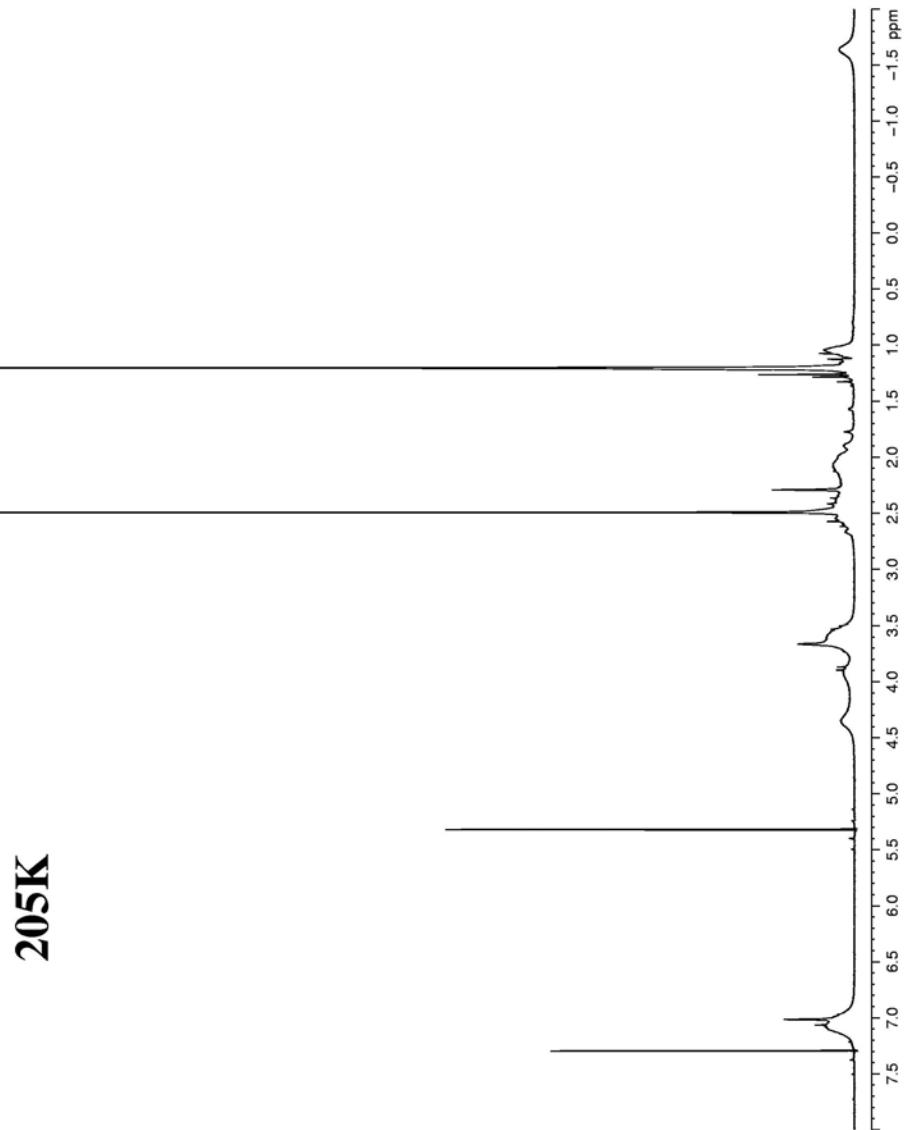
215K



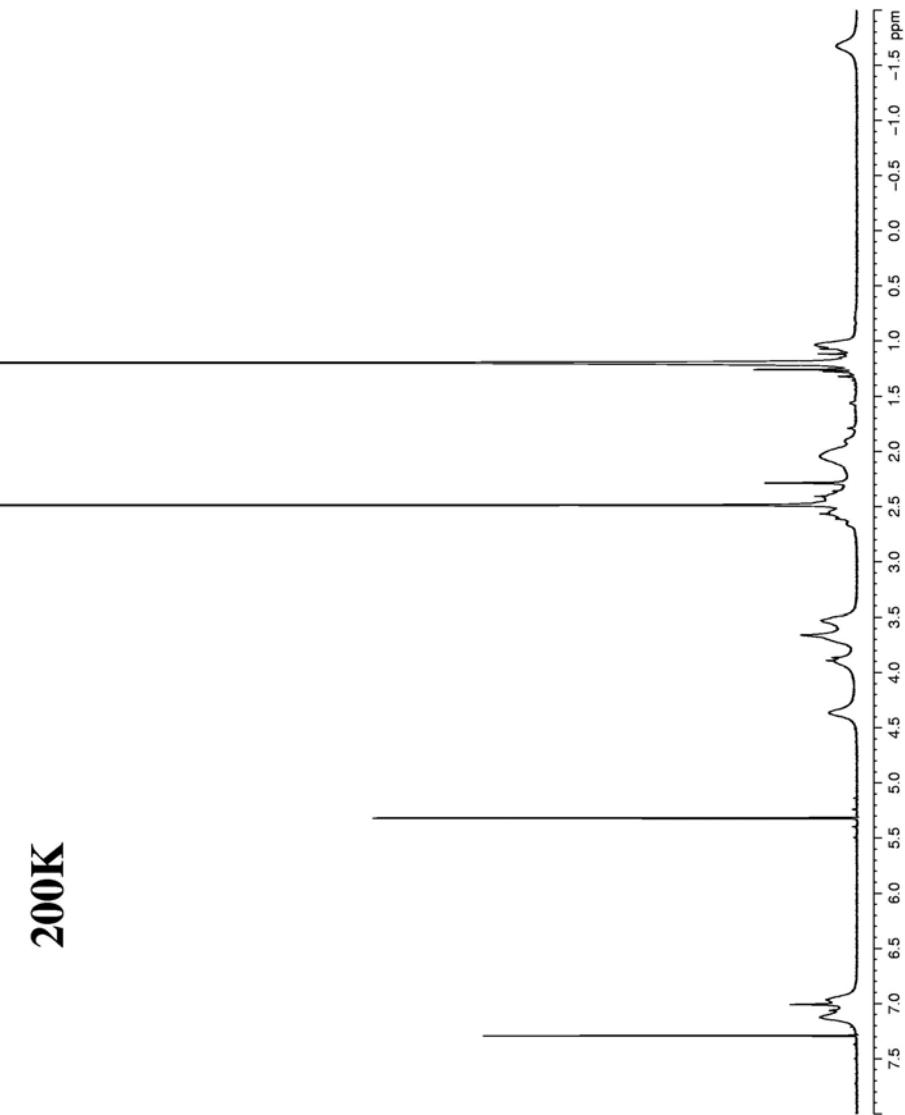
¹H NMR spectrum of **2** at 210K in 3:1 CD₂Cl₂:CDCl₃



¹H NMR spectrum of **2** at 205K in 3:1 CD₂Cl₂:CDCl₃

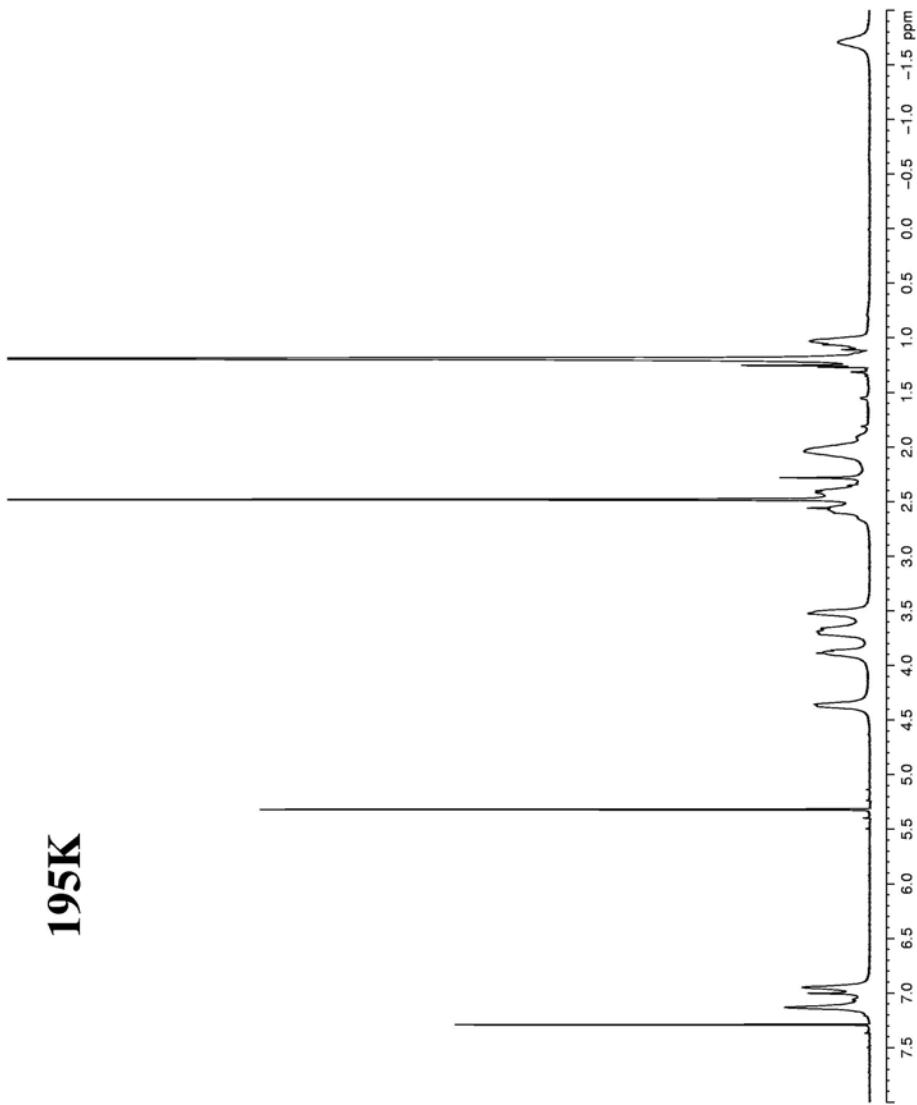


^1H NMR spectrum of **2** at 200K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$



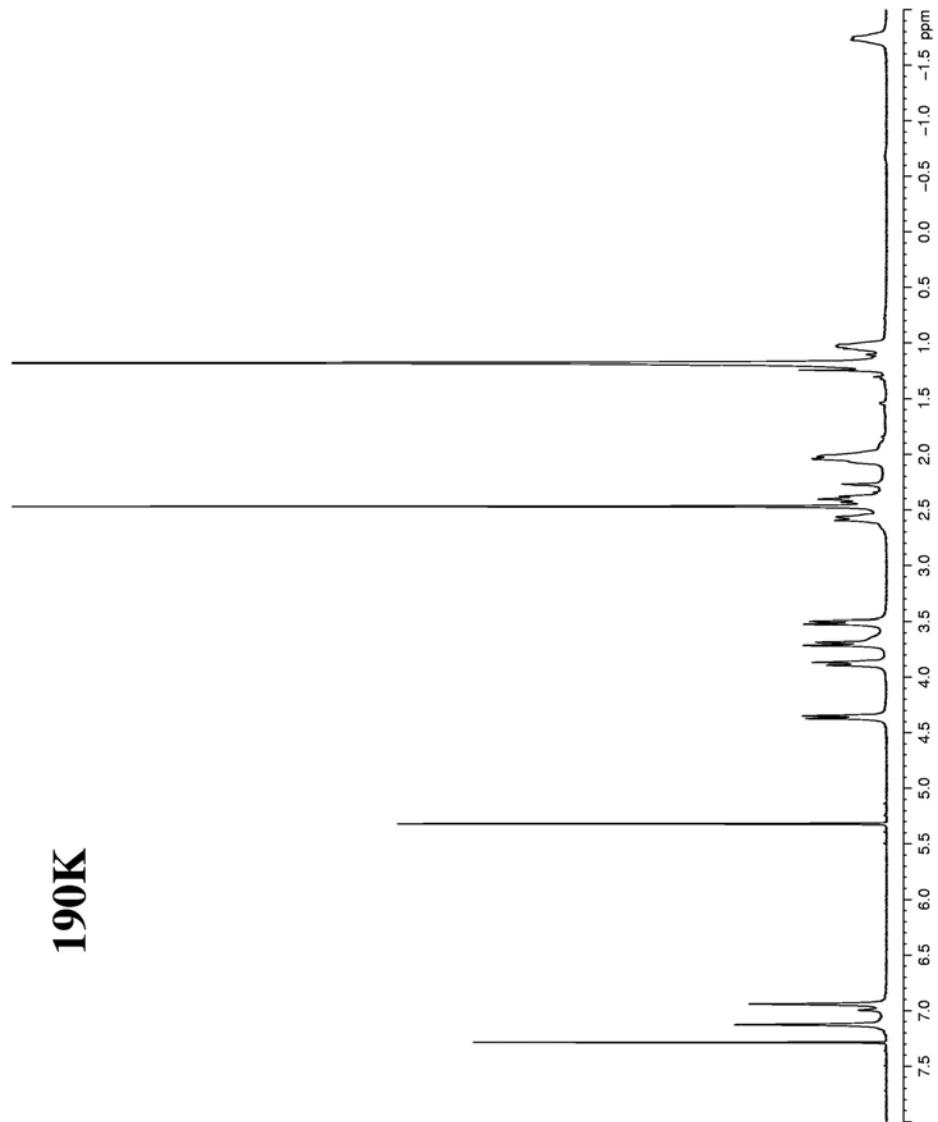
¹H NMR spectrum of **2** at 195K in 3:1 CD₂Cl₂:CDCl₃

195K

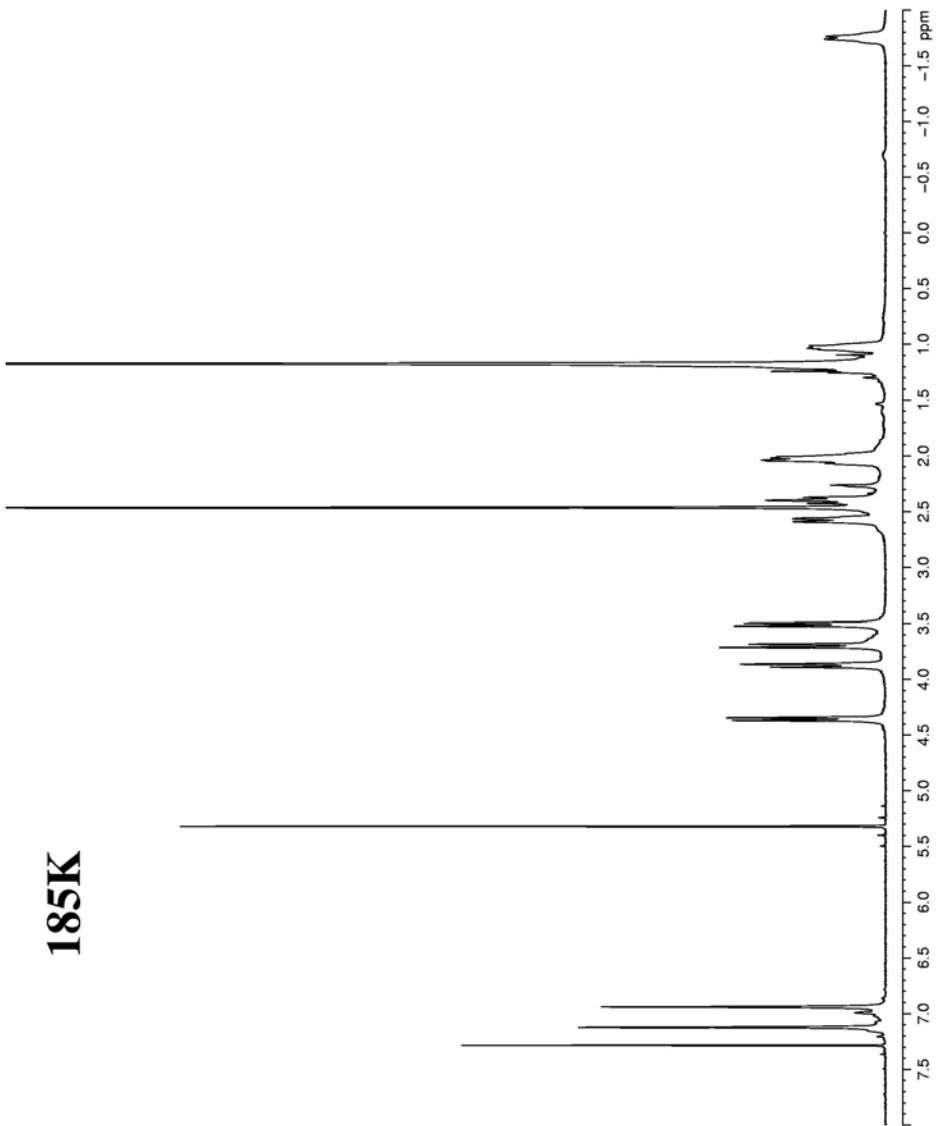


S(I)40

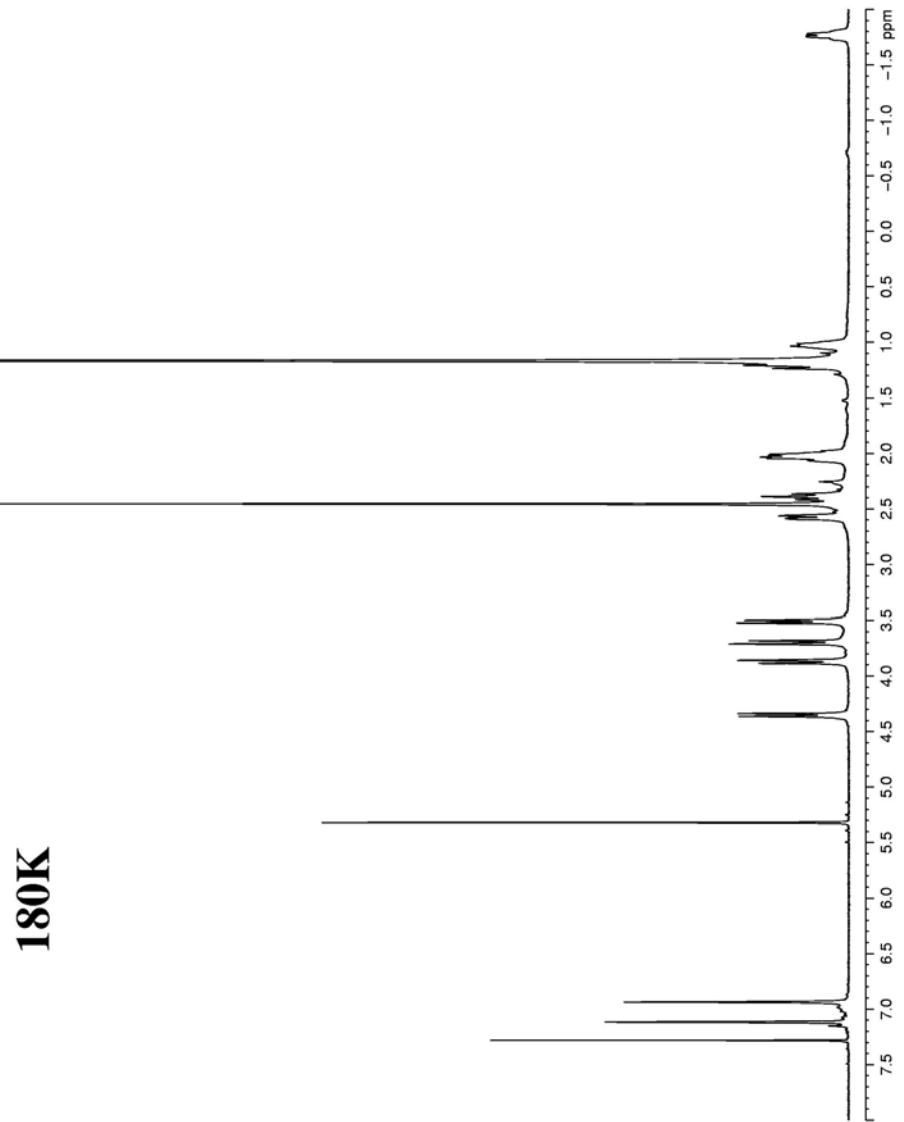
¹H NMR spectrum of **2** at 190K in 3:1 CD₂Cl₂:CDCl₃



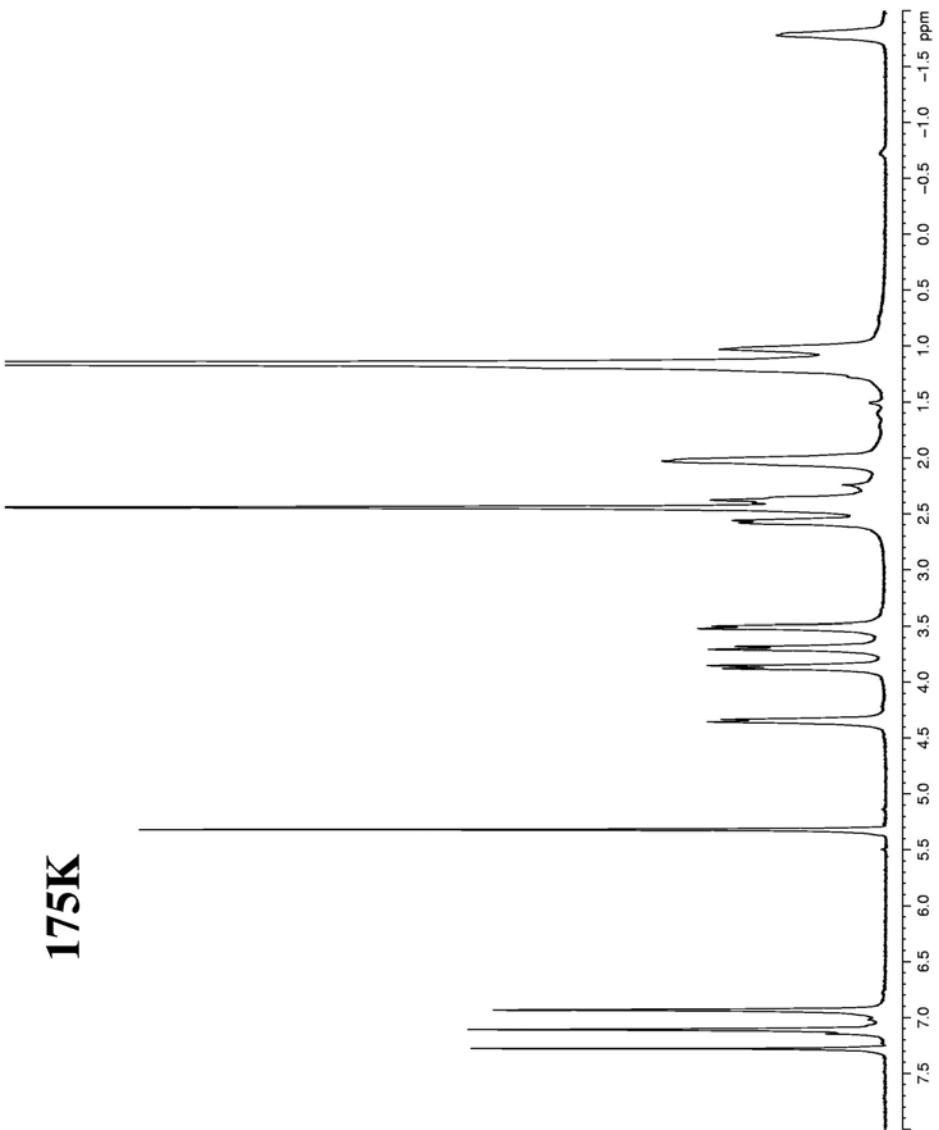
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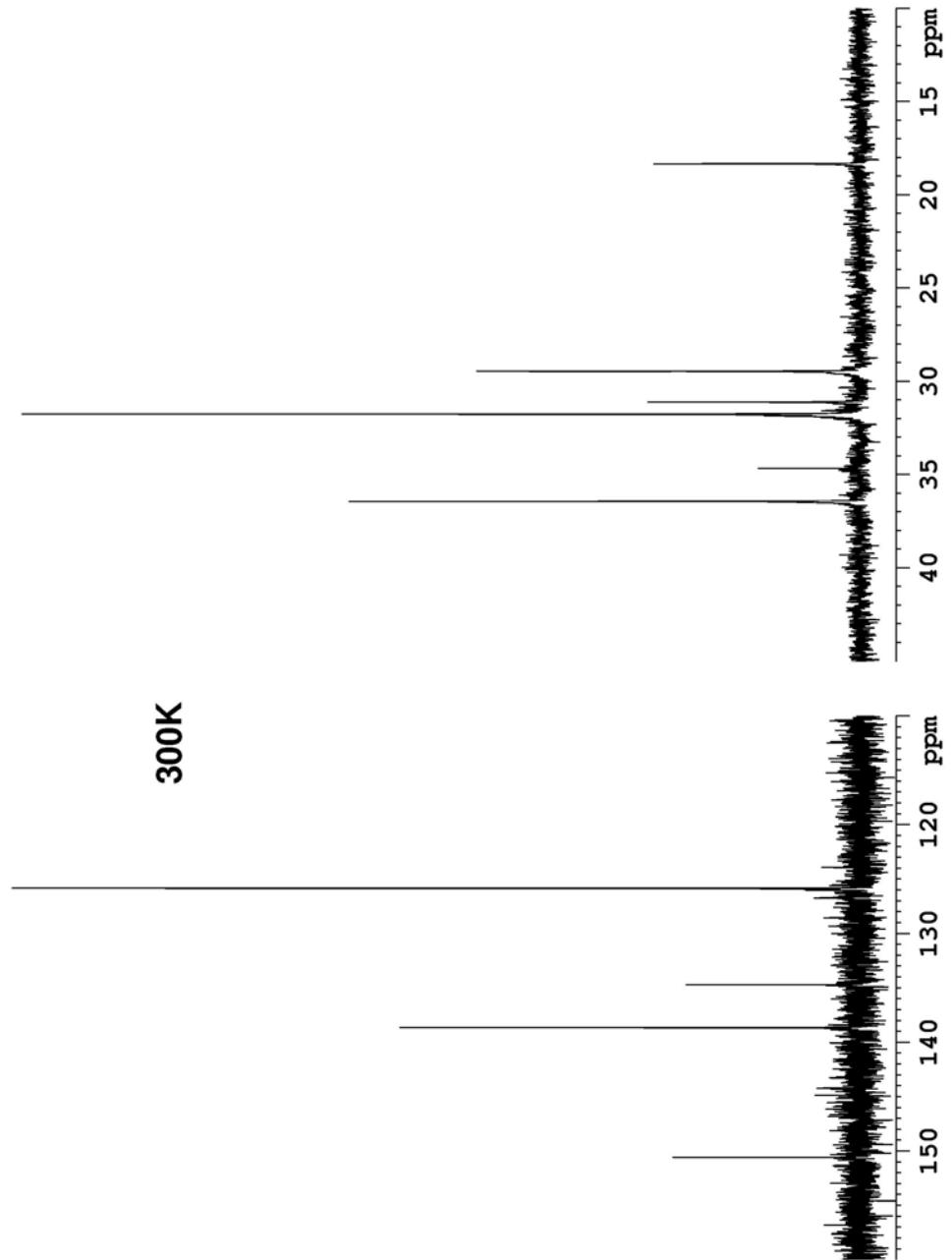
¹H NMR spectrum of **2** at 180K in 3:1 CD₂Cl₂:CDCl₃



¹H NMR spectrum of **2** at 175K in 3:1 CD₂Cl₂:CDCl₃

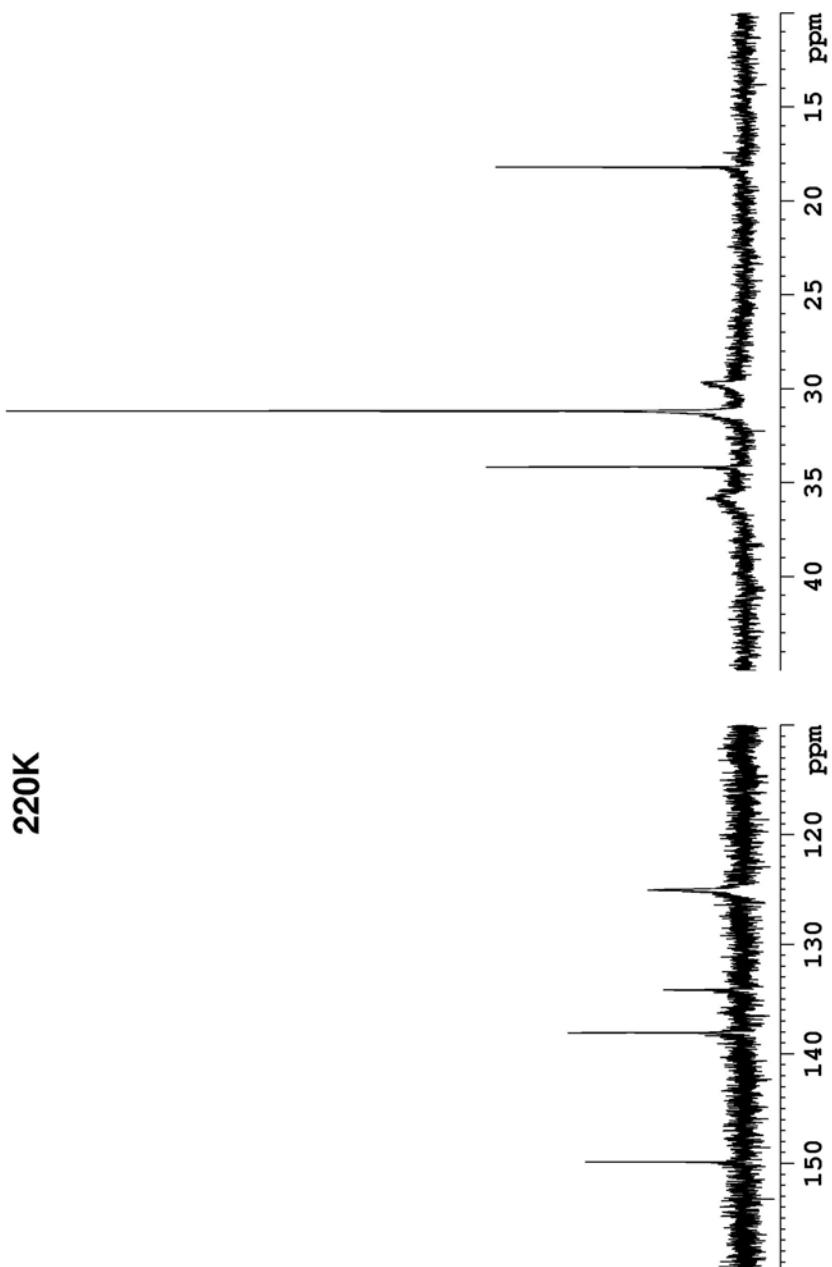


^{13}C NMR spectrum of **2** at 300K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$



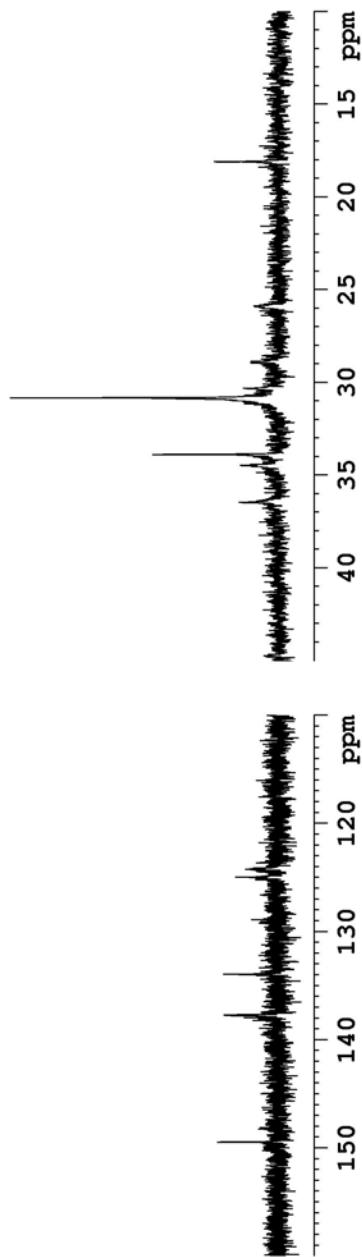
S(I)45

^{13}C NMR spectrum of **2** at 220K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$



^{13}C NMR spectrum of **2** at 190K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$

190K



^{13}C NMR spectrum of **2** at 180K in 3:1 $\text{CD}_2\text{Cl}_2:\text{CDCl}_3$

