

REFERENCES

1. การปิโตรเลียมแห่งประเทศไทย. ส่วนควบคุมคุณภาพและส่วนบริการเทคนิคตลาดพาณิชย์. **ความรู้เกี่ยวกับปิโตรเลียม ฉบับปี 2000**. พิมพ์ครั้งที่ 1. กุมภาพันธ์ 2543.
2. Nikanjam, M. **Low Emissions Diesel Fuel**, US. Patent No. 5,389,111, Feb. 14, 1995.
3. Hobson, G.D. **Modern Petroleum Technology Part 2**. 5th ed. New York: John Wiley & Sons, 1984, pp.823-828
4. ศูนย์วิจัยและพัฒนา การปิโตรเลียมแห่งประเทศไทย. **หนังสือชุดปิโตรเลียมความรู้** พิมพ์ครั้งที่ 1, 2539, หน้า 2, 13, 15
5. Poirer, M.A., Steere, D.V., and Krogh, J.A. **Cetane Improver Compositions Comprising Nitrated Fatty Acid Derivatives**. US Patent 5,454,842, 1995.
6. Purcell, R.F., and Hallock, L.L. **Cetane Improver for Diesel Fuel**. US Patent 4,549,883, 1985.
7. Suppes, G.J. et al. Synthesis and Cetane Improver Performance of Fatty Acid Glycol Nitrates. **Fuel** 1999, Vol.78, pp. 73-81.
8. Von Schickh, O., **Production of Cycloaliphatic Nitrates**, US. Patent No. 3,301,891, Jan. 31, 1967.
9. Filbey, A.H. **Diesel Fuel Composition**. US. Patent No. 4,406,665, Sep. 27, 1983.
10. Russel, T.J. Additives influencing diesel fuel combustion. **Gasoline and Diesel Fuel Additives**. New York: John Wiley & Sons, 1989, pp. 65-88.
11. The American Society of Mechanical Engineers. **Diesel Fuel Oils Production, Characteristics, and Combustion**. New York: 1947, pp. 59, 78-79, 88-89.

12. Virgil, B.G. **Petroleum Products Handbook**. 1st ed. New York: McGraw-Hill, 1960, pp. 6-2 - 6-11.
13. Patberg, J.B. **Petroleum & Chemical Processes**. Exxon Research and Engineering Company, 1976.
14. Popovich, M. **Fuels and Lubricants**. London: John Wiley & Sons, 1959, pp. 134-145.
15. Schobert, H.H. **The Chemistry of Hydrocarbon Fuels**. 2nd ed. London: Butterworth-Heinemann, 1991, pp. 197-202.
16. Allinson, J.P. **Criteria for Quality of Petroleum Products**. 1st ed. Great Britain: Applied Science Publishers, 1975, pp. 121-141.
17. Collins, J.M., and Unzelman, G.H. Better cetane prediction equations developed. **Oil & Gas Journal**. June 7, 1982, pp. 148-160.
18. Society of Automotive Engineers (SAE), **SAE Fuels and Lubricants Standards Manual**. 1995, pp. 49-63.
19. Liotta, Jr. et al. **Diesel Fuel Composition**. US. Patent No. 5,258,049, Nov. 2, 1993.
20. Siraprapakit, S. **Synthesis of Dinitrate Compounds from Alkane Diols as Cetane Improver**. Master's Thesis, Program of Petrochemistry and Polymer Science, Graduate School, Chulalongkorn University, 2000.
21. Suttipitakwong, C. **Synthesis of Dinitrate Compounds from Alkylene Glycols as Cetane Improver**. Master's Thesis, Program of Petrochemistry and Polymer Science, Graduate School, Chulalongkorn University, 2000.

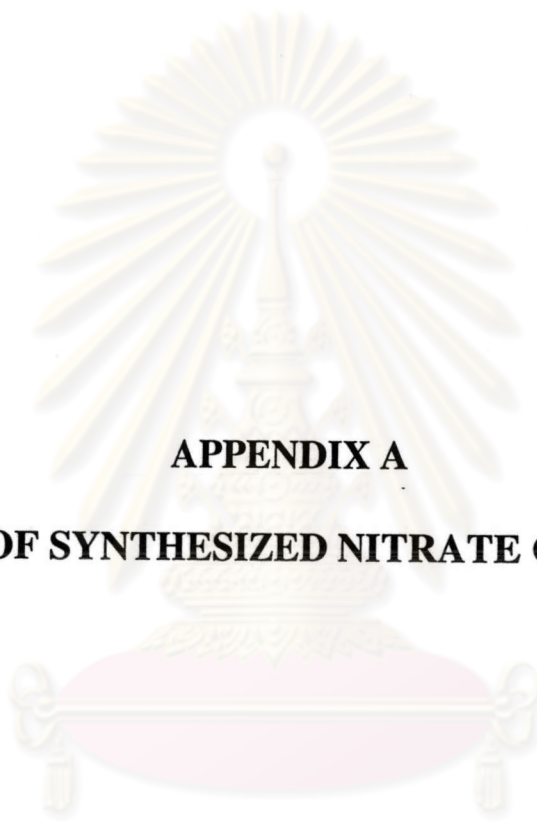
22. Vasaruchtragul, J. **Synthesis of Dinitrate Compounds as Cetane Number Improver**. Master's Thesis, Program of Petrochemistry and Polymer Science, Graduate School, Chulalongkorn University, 1997.
23. Kornblum, N. and Teittlbaum, C. The Basis for the Report that Rearrangements Occur when Cyclopentyl Iodide and Cyclohexyl Iodide React with Silver Nitrite. **Journal of American Chemical Society**. Vol.74, pp. 3076-3078.
24. Clothier, P., Aguda, B., Moise, A., and Pritchard, H. How do Diesel Fuel Ignition Improvers Works?. **Chemical Society Reviews**, 1993, pp. 101-108.
25. Anthony, J.S., **Process for the Manufacture of Nitric Acid Esters**. US Patent 4,853,157, 1989.
26. Sadtler Standard ^{13}C -NMR Spectra Vol. 11, 12, 13, pp.2138
27. Sadtler Standard ^{13}C -NMR Spectra Vol. 9, 10, pp.1416
28. The Aldrich Library of FT-NMR Spectra 2 ed. Vol. 1, pp.244
29. The Aldrich Library of FT-NMR Spectra 2 ed. Vol. 1, pp.384
30. The Aldrich Library of FT-NMR Spectra 2 ed. Vol. 1, pp.622
31. Sadtler Standard ^{13}C -NMR Spectra Vol. 1, 2, 3, pp.214

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APPENDICES

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APPENDIX A

SPECTRA OF SYNTHESIZED NITRATE COMPOUNDS

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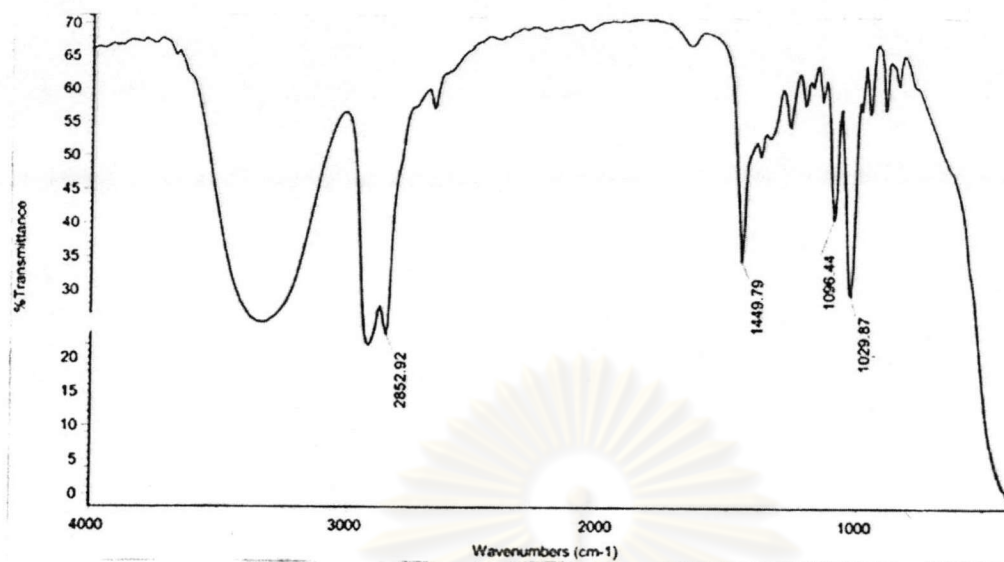


Figure A1 FTIR Spectrum of Cyclohexylmethanol (NaCl)

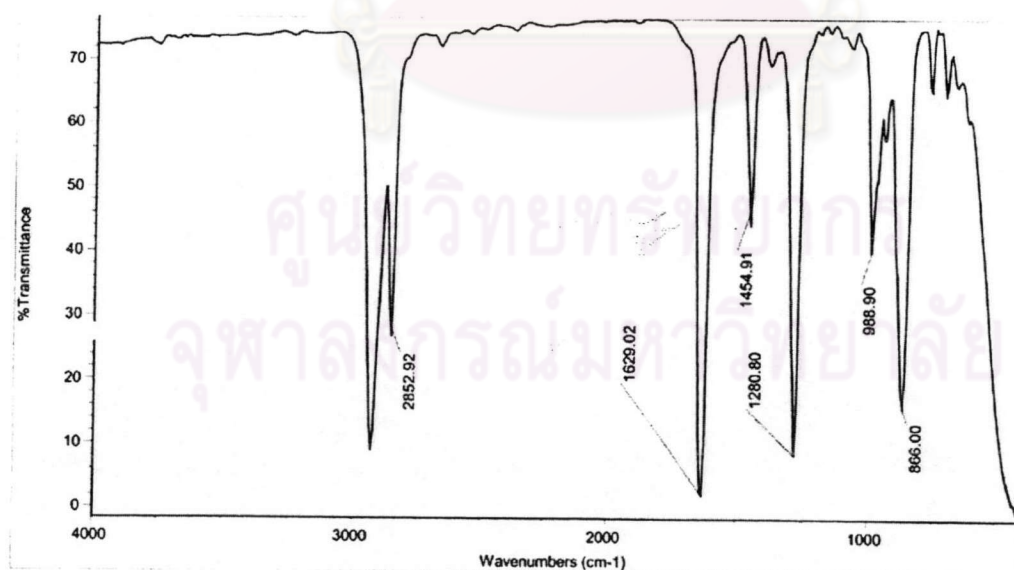


Figure A2 FTIR Spectrum of Cyclohexylmethyl Nitrate (NaCl)

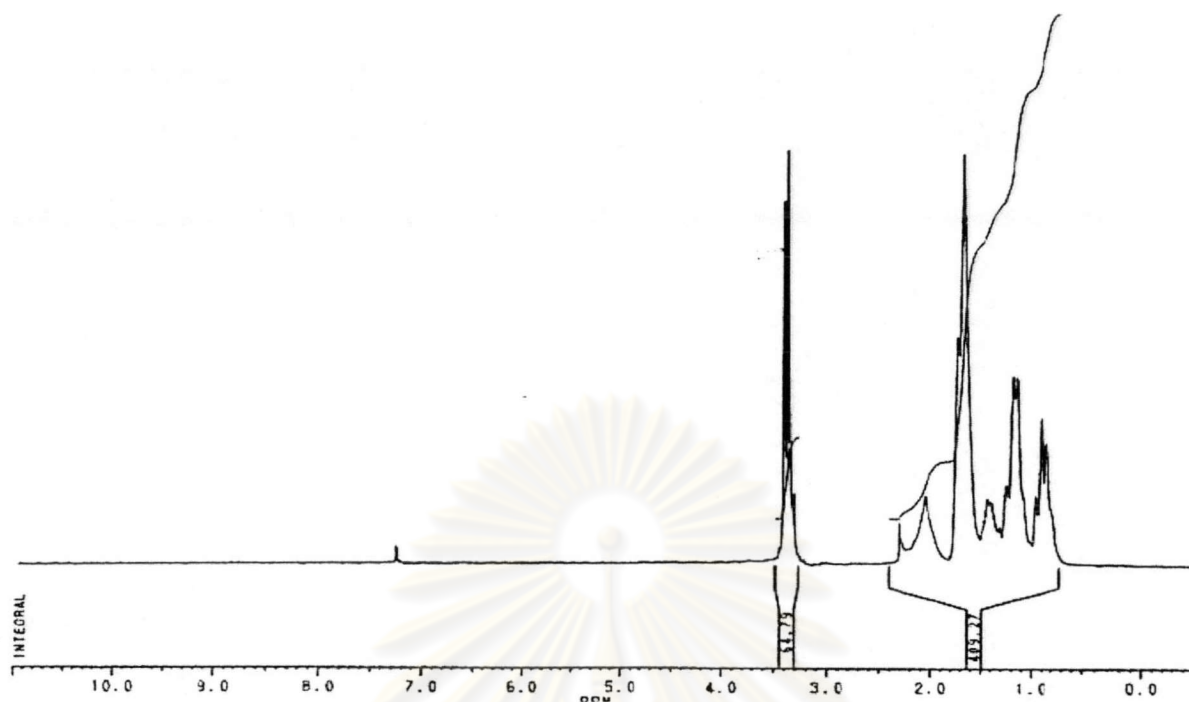


Figure A3 $^1\text{H-NMR}$ Spectrum of Cyclohexylmethanol (CDCl_3)

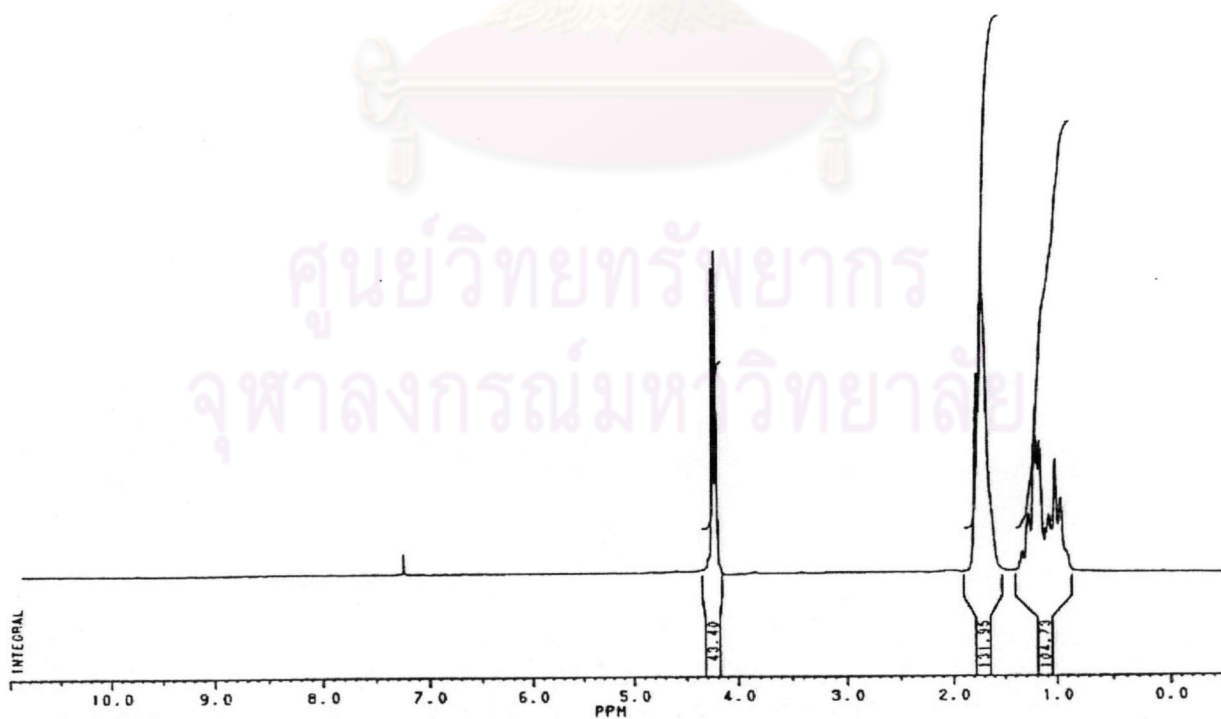


Figure A4 $^1\text{H-NMR}$ Spectrum of Cyclohexylmethyl Nitrate (CDCl_3)

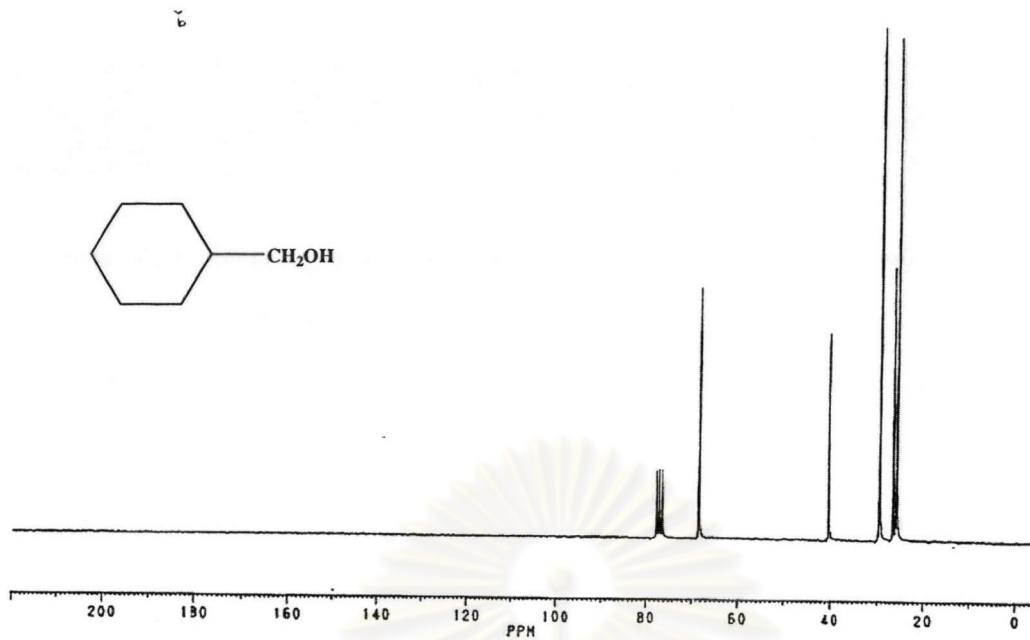


Figure A5 ^{13}C -NMR Spectrum of Cyclohexylmethanol (CDCl_3)

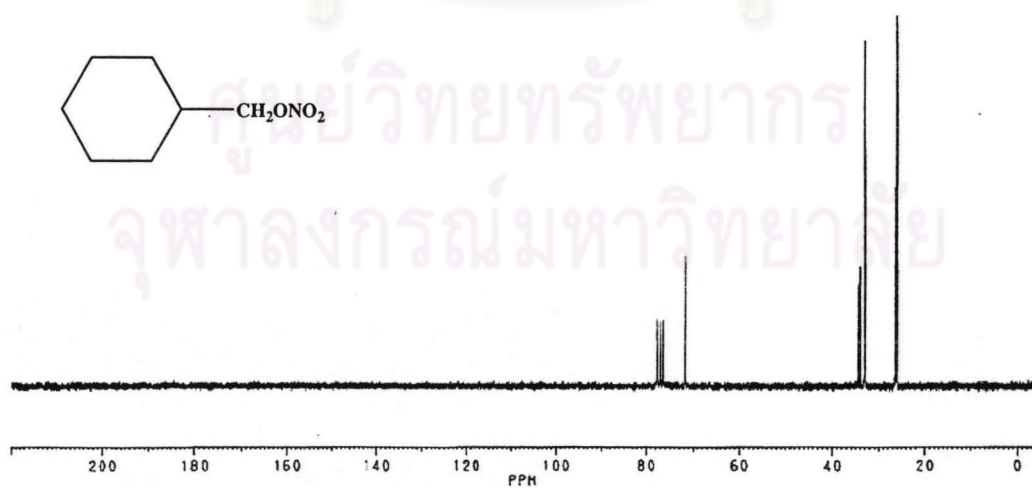


Figure A6 ^{13}C -NMR Spectrum of Cyclohexylmethyl Nitrate (CDCl_3)

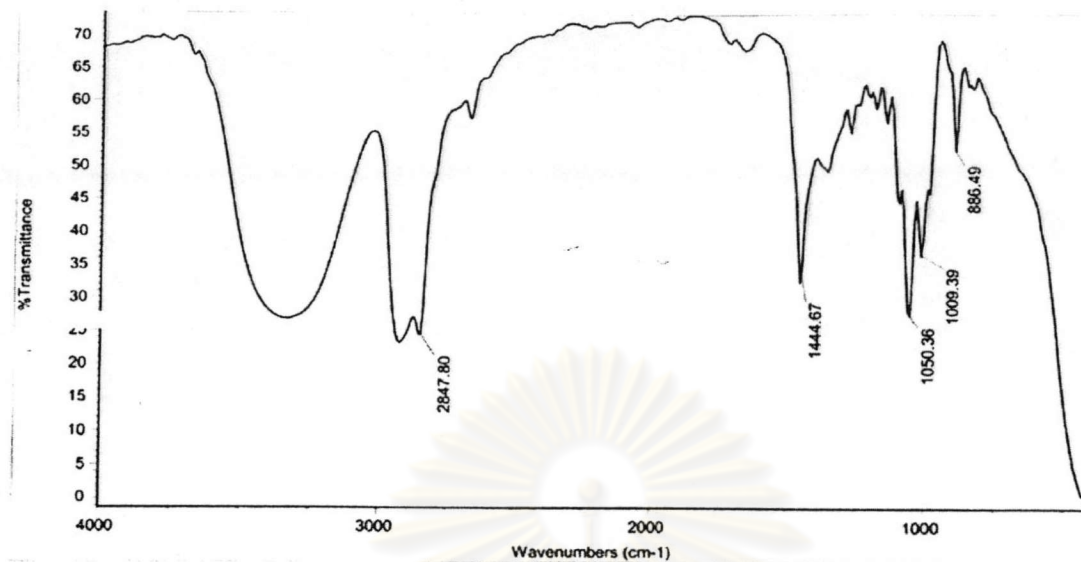


Figure A7 FTIR Spectrum of 2-Cyclohexylethanol (NaCl)

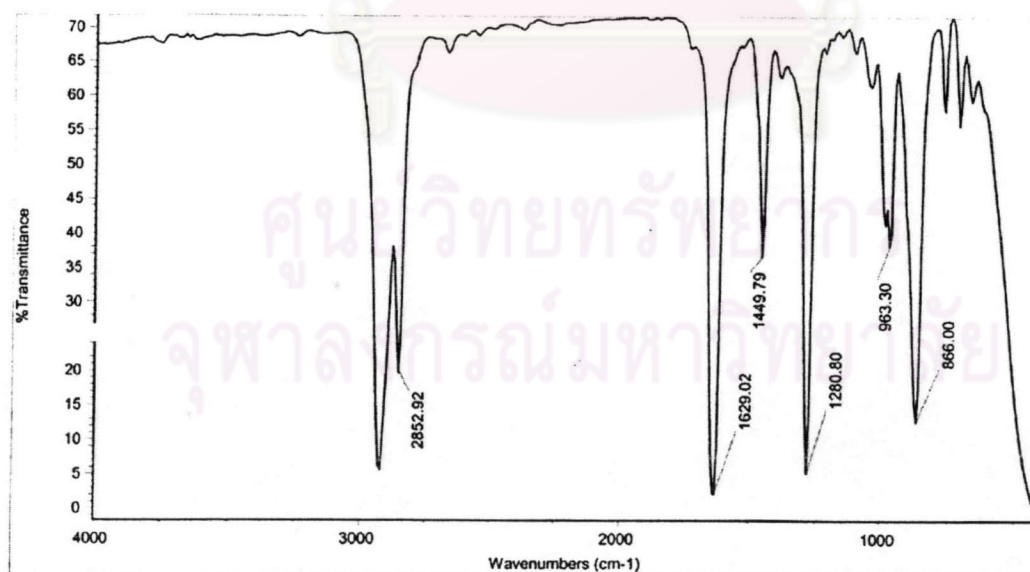


Figure A8 FTIR Spectrum of 2-Cyclohexylethyl Nitrate (NaCl)

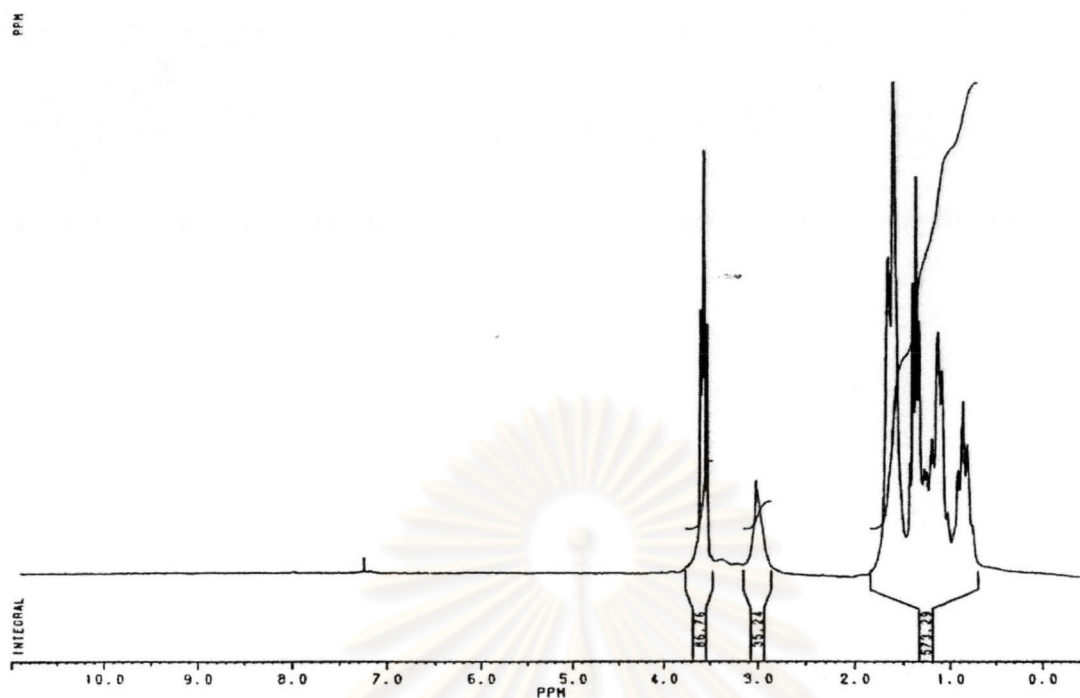


Figure A9 ¹H-NMR Spectrum of 2-Cyclohexylethanol (CDCl₃)

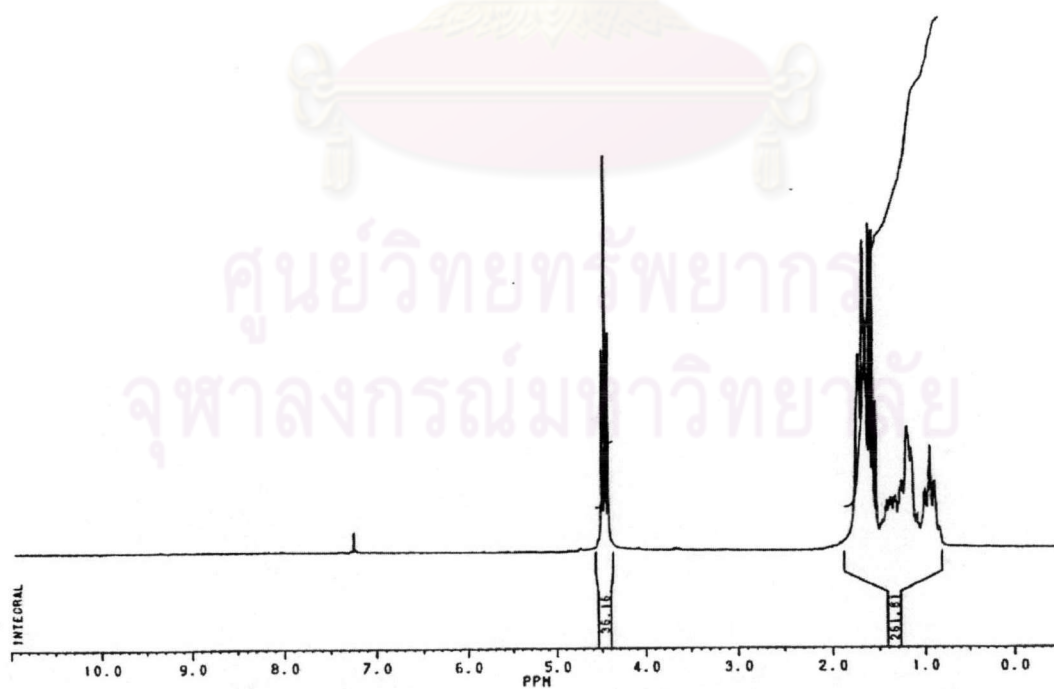


Figure A10 ¹H-NMR Spectrum of 2-Cyclohexylethyl Nitrate (CDCl₃)

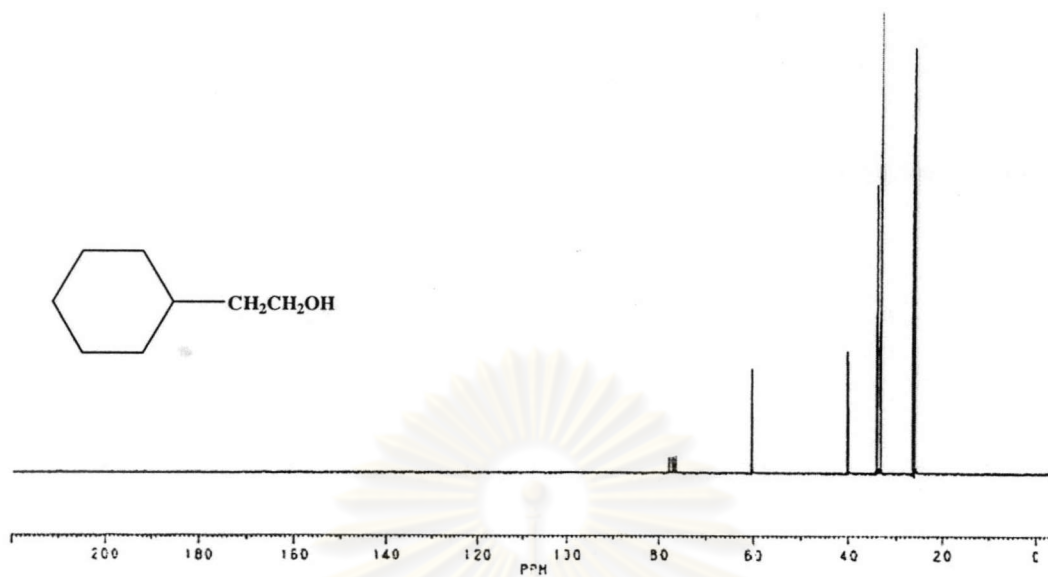


Figure A11 ^{13}C -NMR Spectrum of 2-Cyclohexylethanol (CDCl_3)

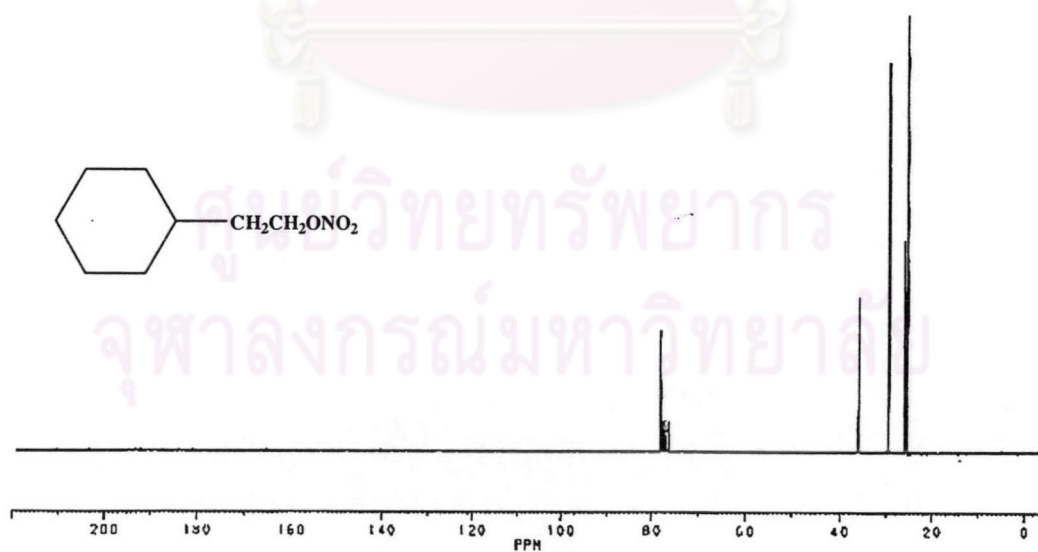


Figure A12 ^{13}C -NMR Spectrum of 2-Cyclohexylethyl Nitrate (CDCl_3)

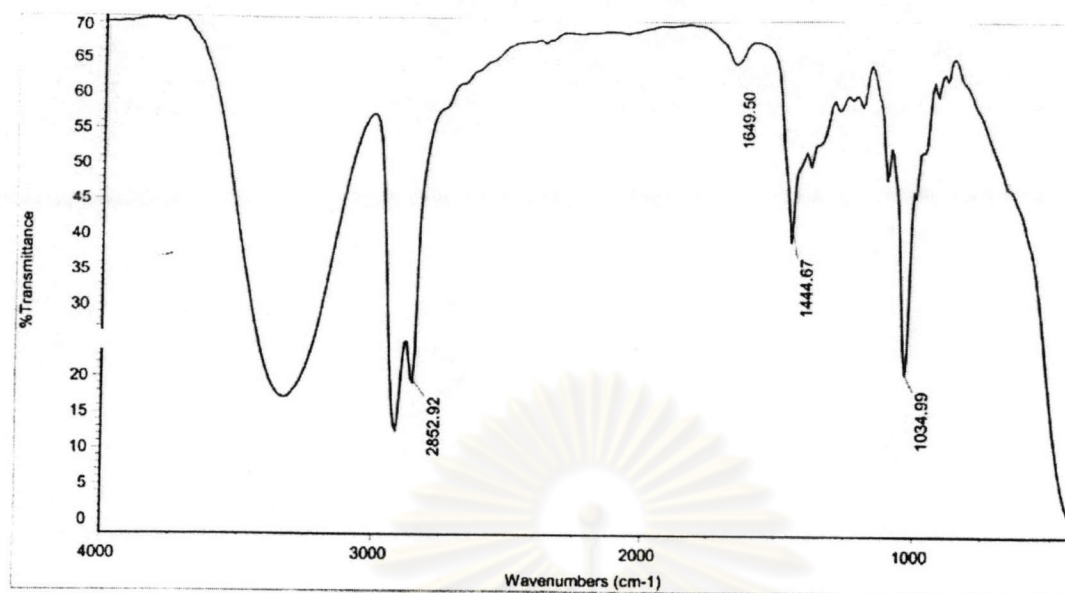


Figure A13 FTIR Spectrum of 1,4-Cyclohexanedimethanol (NaCl)

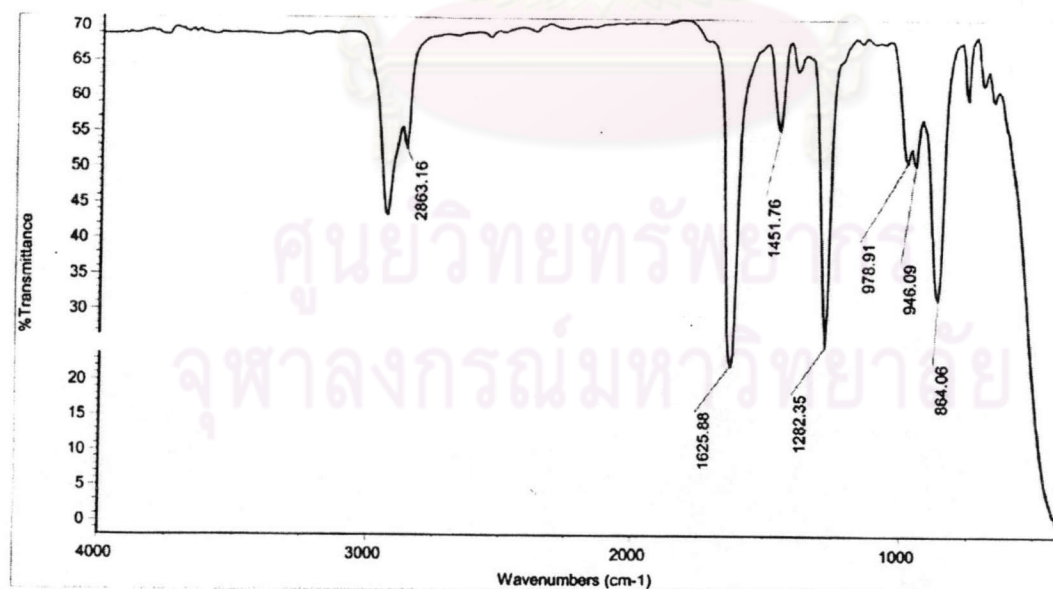


Figure A14 FTIR Spectrum of 1,4-Cyclohexanedimethyl Nitrate (NaCl)

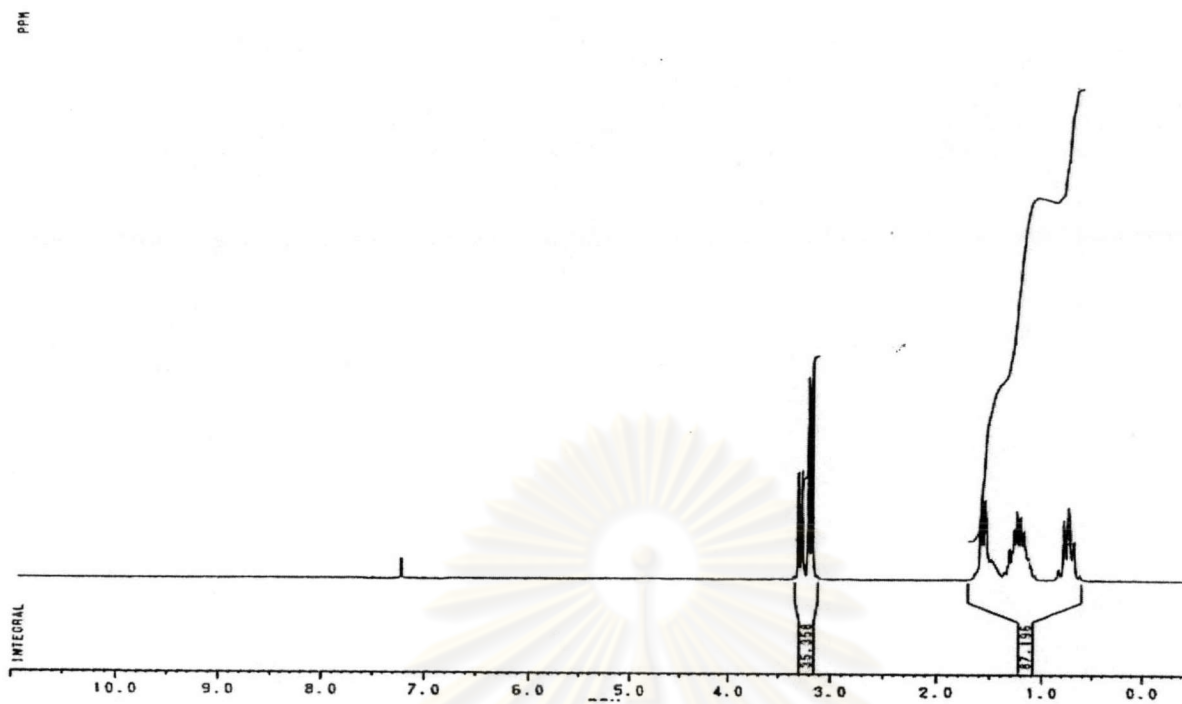


Figure A15 $^1\text{H-NMR}$ Spectrum of 1,4-Cyclohexanedimethanol (CDCl_3)

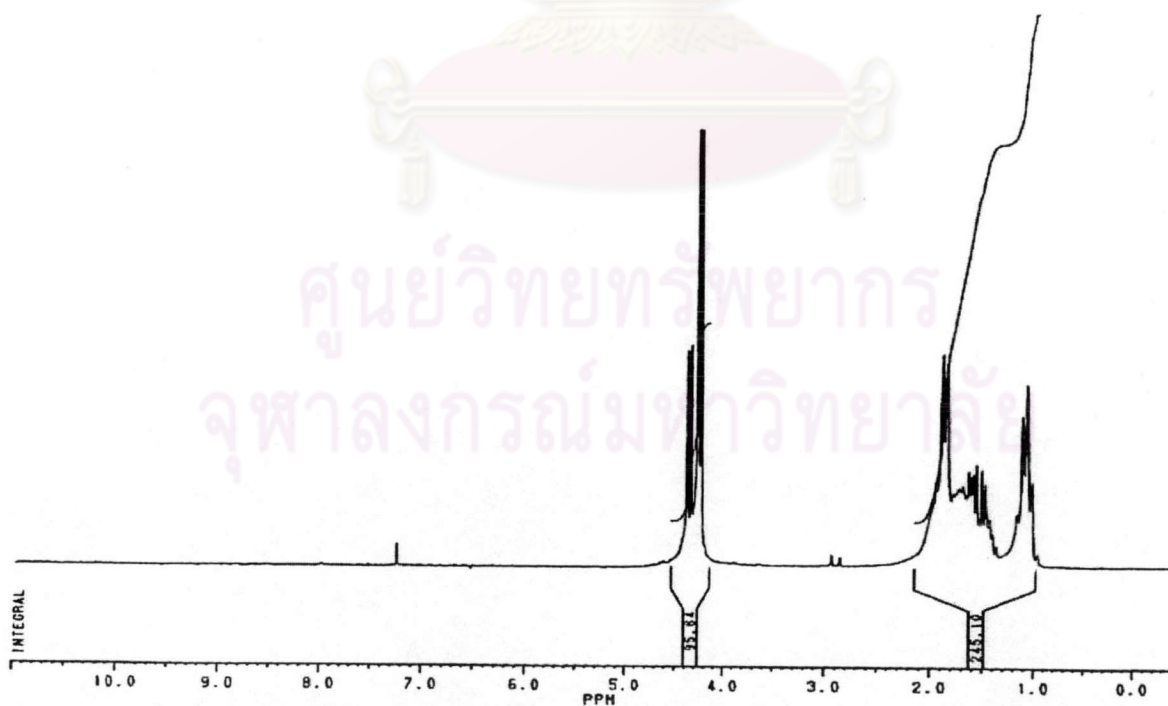


Figure A16 $^1\text{H-NMR}$ Spectrum of 1,4-Cyclohexanedimethyl Nitrate (CDCl_3)

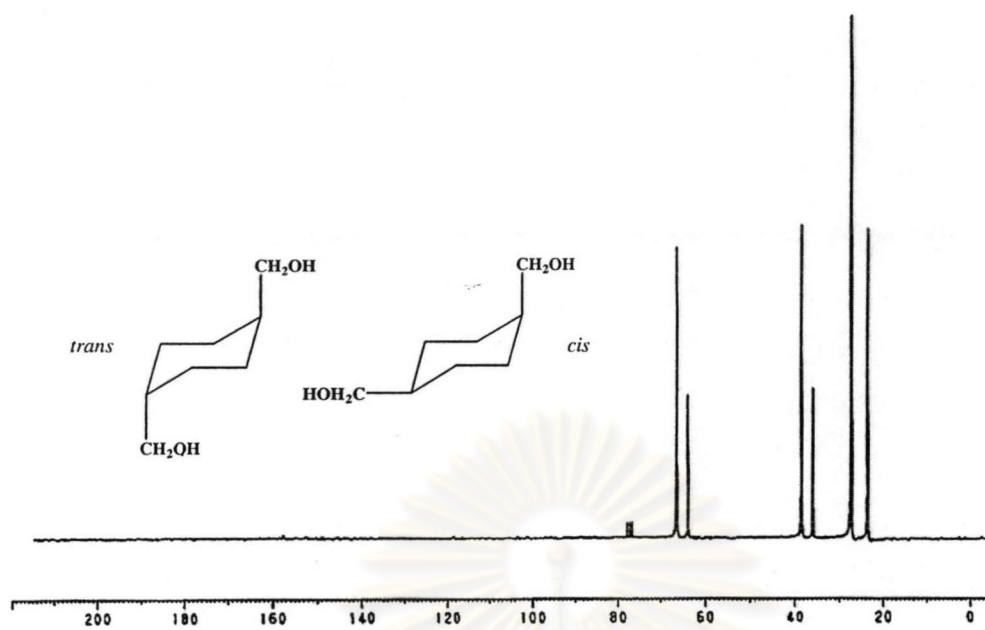


Figure A17 ^{13}C -NMR Spectrum of 1,4-Cyclohexanedimethanol (CDCl_3)

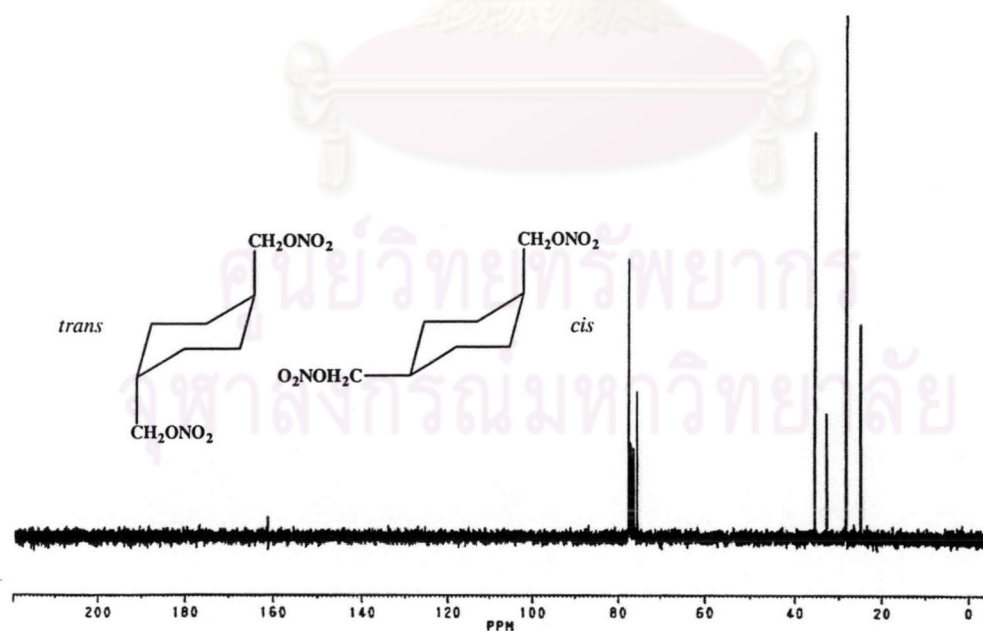


Figure A18 ^{13}C -NMR Spectrum of 1,4-Cyclohexanedimethyl Nitrate (CDCl_3)

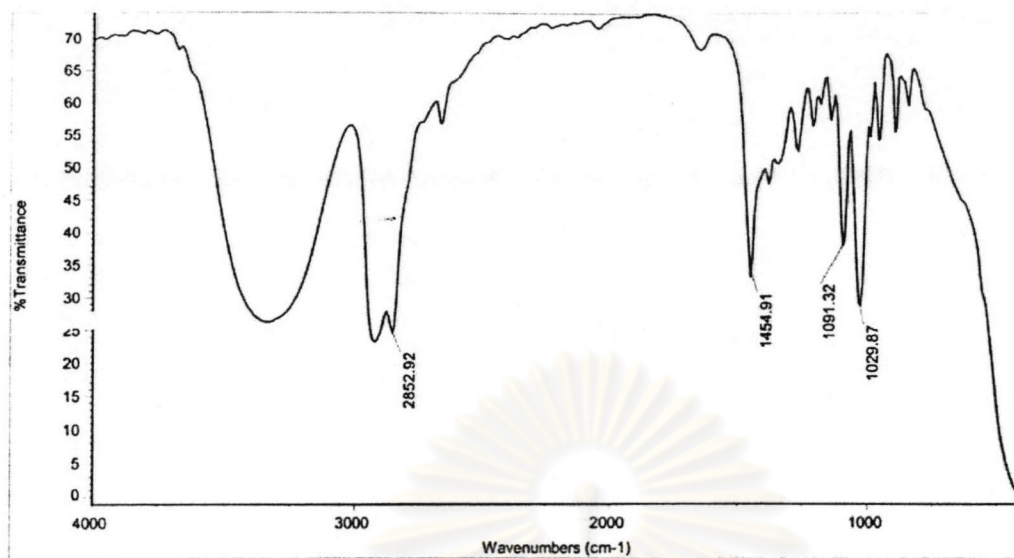


Figure A19 FTIR Spectrum of Tetrahydrofurfuryl Alcohol (NaCl)

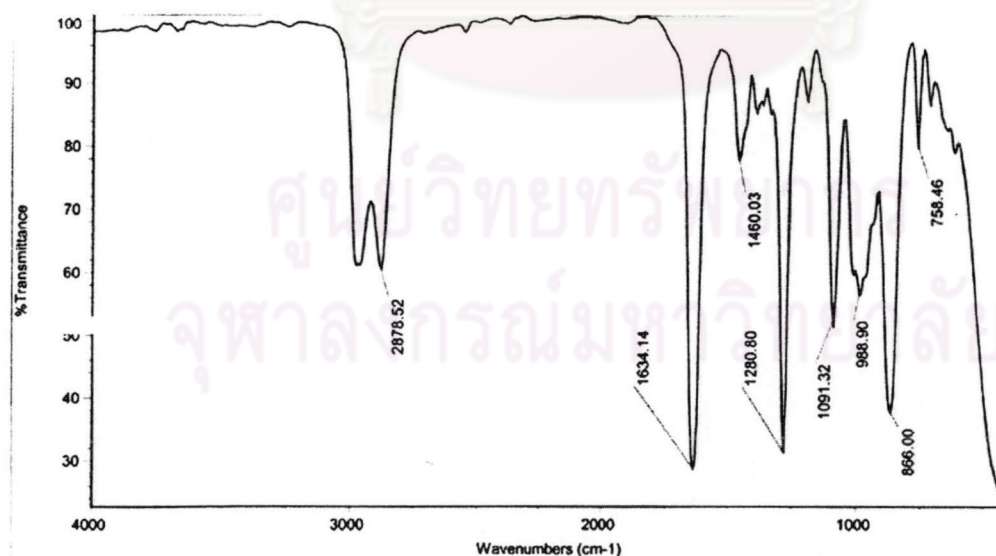


Figure A20 FTIR Spectrum of Tetrahydrofurfuryl Nitrate (NaCl)

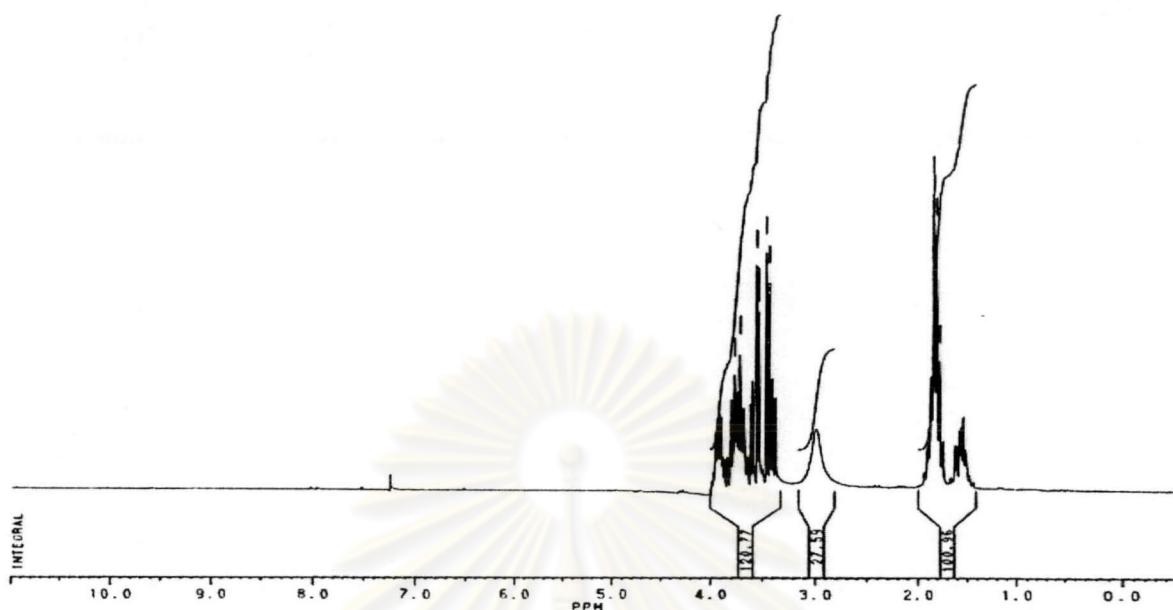


Figure A21 $^1\text{H-NMR}$ Spectrum of Tetrahydrofurfuryl Alcohol (CDCl_3)

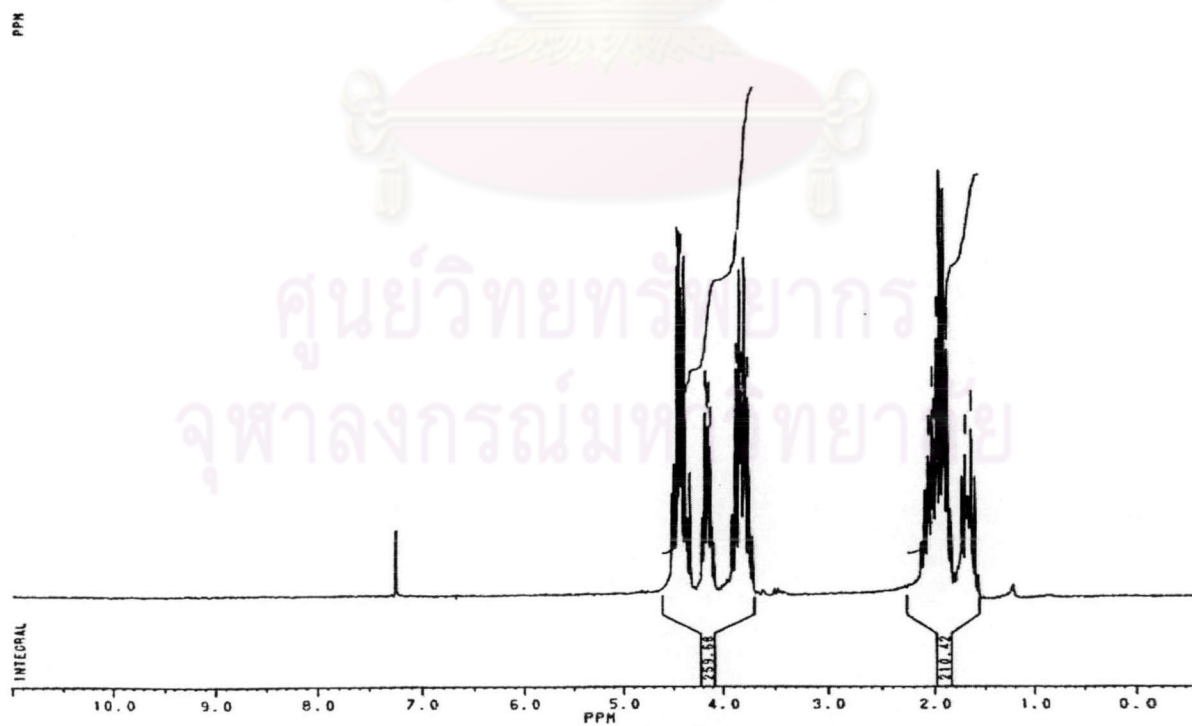


Figure A22 $^1\text{H-NMR}$ Spectrum of Tetrahydrofurfuryl Nitrate (CDCl_3)

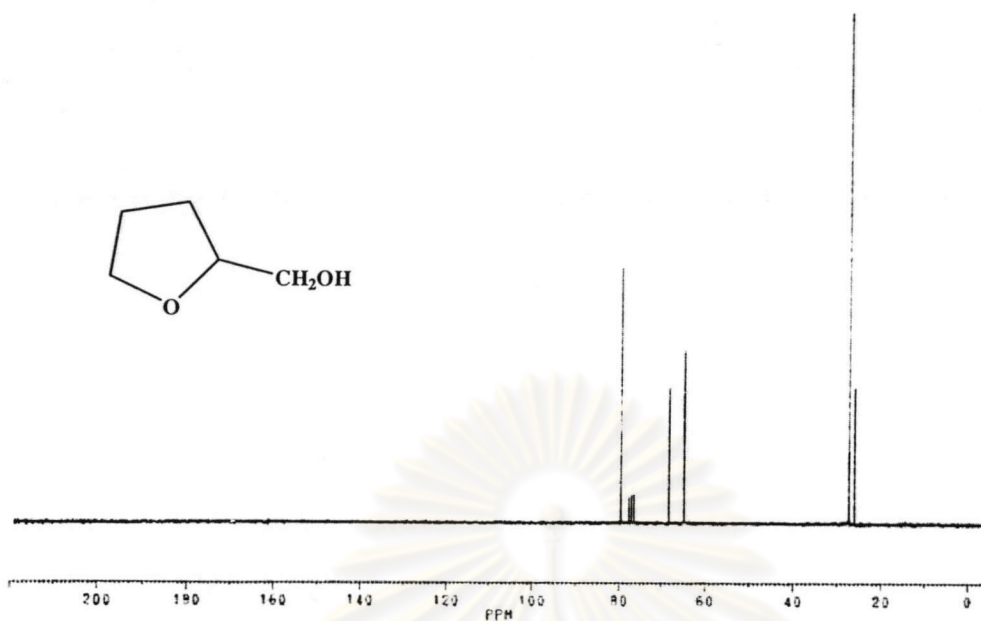


Figure A23 ^{13}C -NMR Spectrum of Tetrahydrofurfuryl Alcohol (CDCl_3)

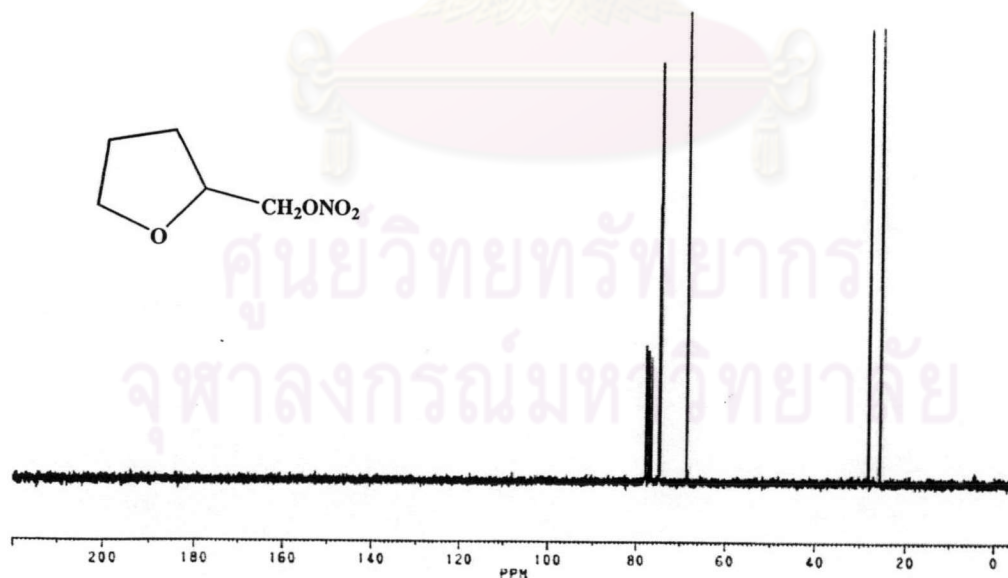


Figure A24 ^{13}C -NMR Spectrum of Tetrahydrofurfuryl Nitrate (CDCl_3)

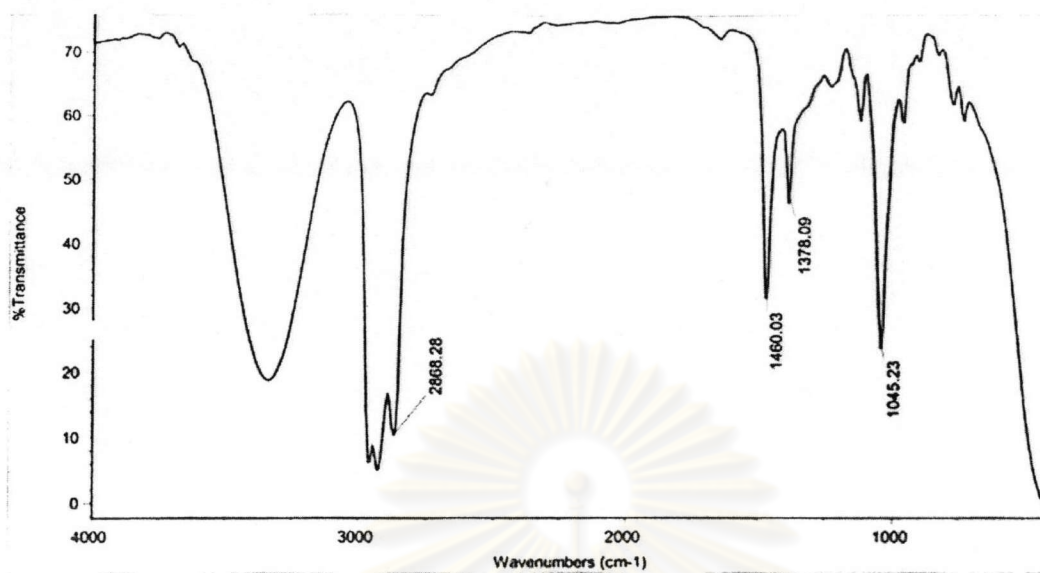


Figure A25 FTIR Spectrum of 2-Ethyl-1-hexanol (NaCl)

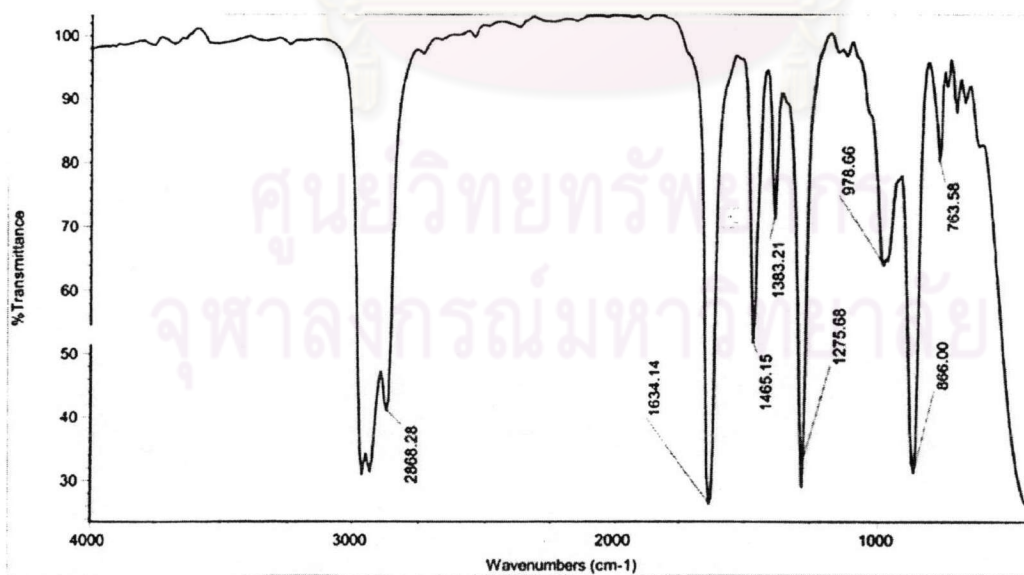


Figure A26 FTIR Spectrum of 2-Ethylhexyl Nitrate (NaCl)

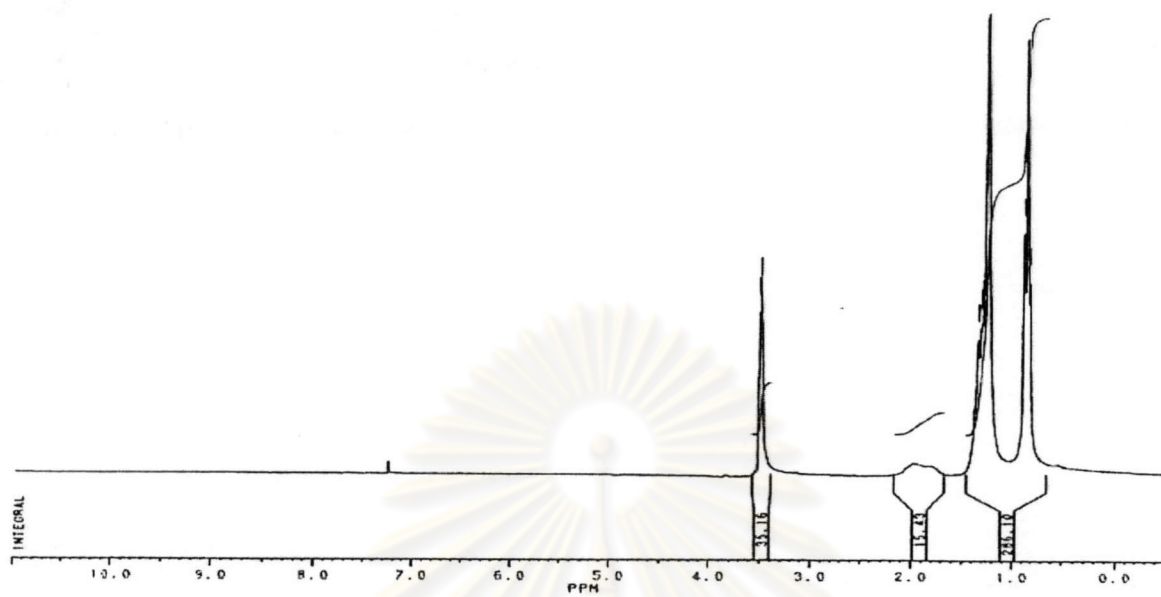


Figure A27 $^1\text{H-NMR}$ Spectrum of 2-Ethyl-1-hexanol (CDCl_3)

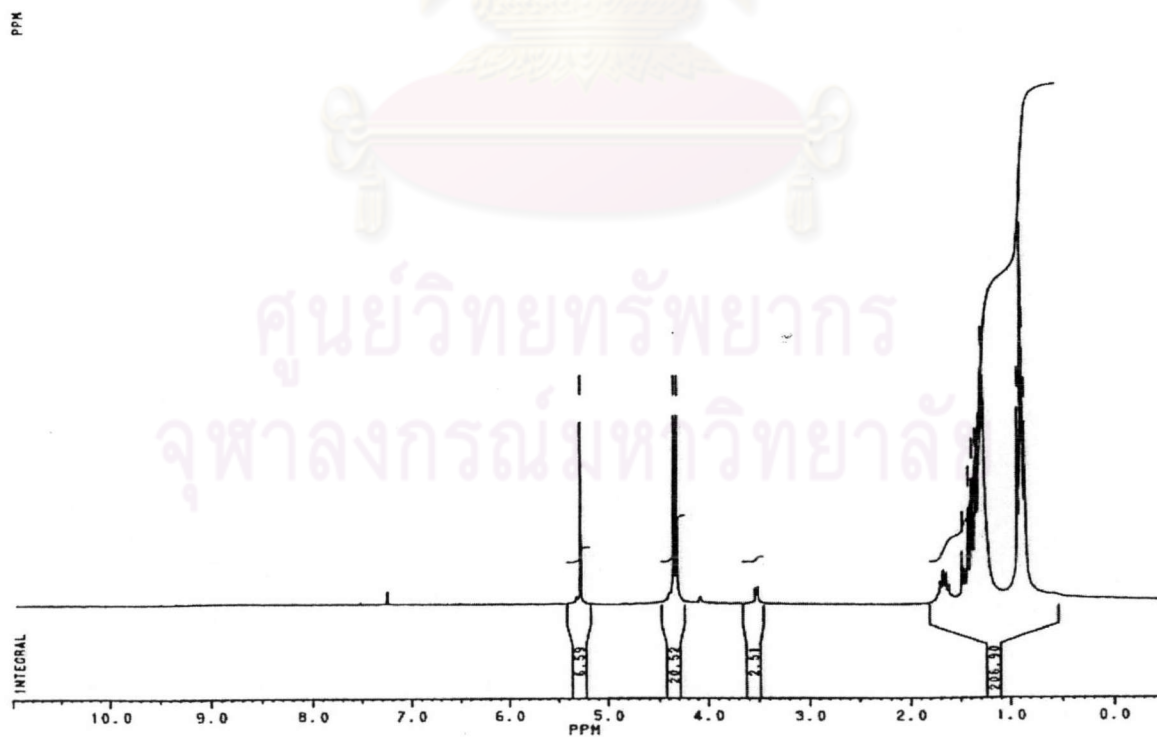


Figure A28 $^1\text{H-NMR}$ Spectrum of 2-Ethylhexyl Nitrate (CDCl_3)

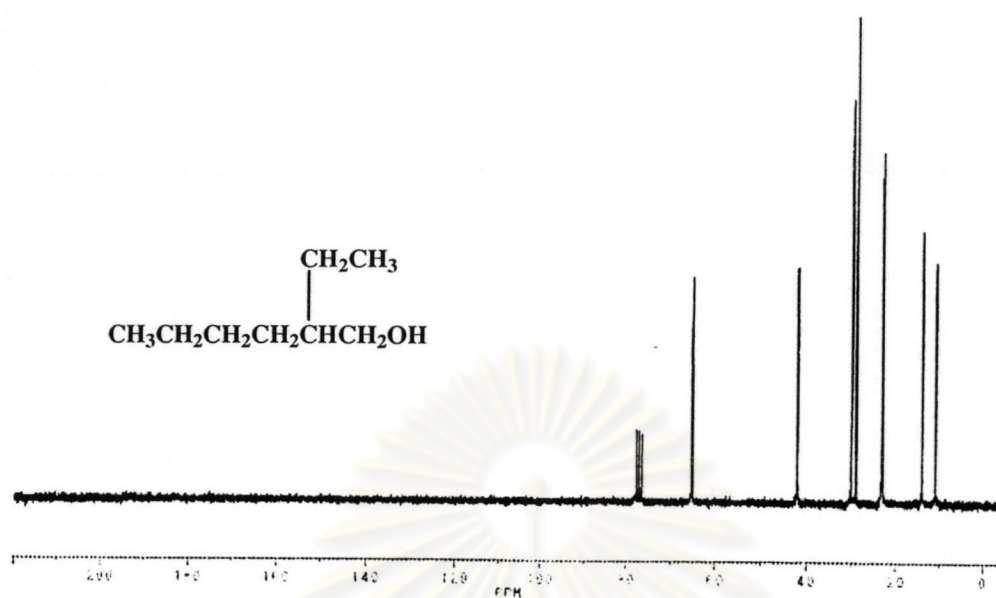


Figure A29 ^{13}C -NMR Spectrum of 2-Ethyl-1-hexanol (CDCl₃)

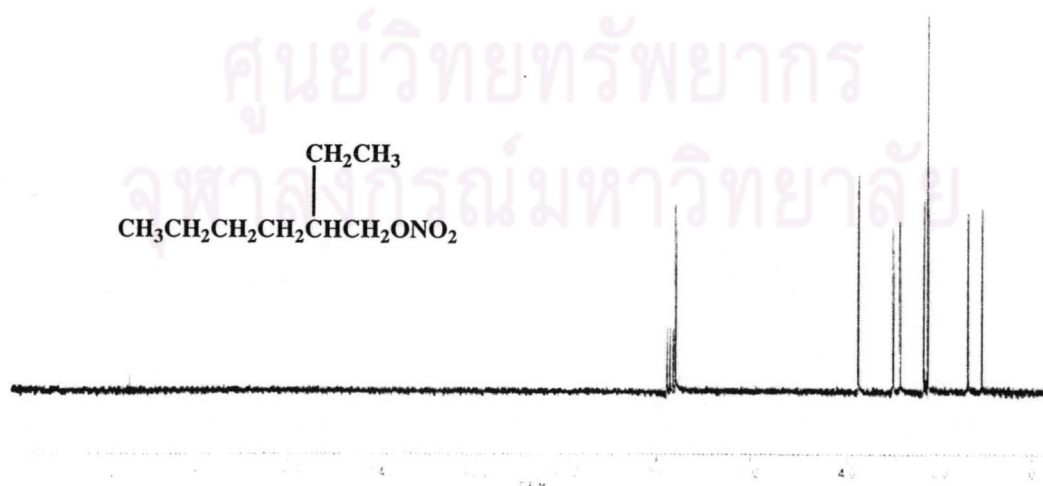


Figure A30 ^{13}C -NMR Spectrum of 2-Ethylhexyl Nitrate (CDCl₃)

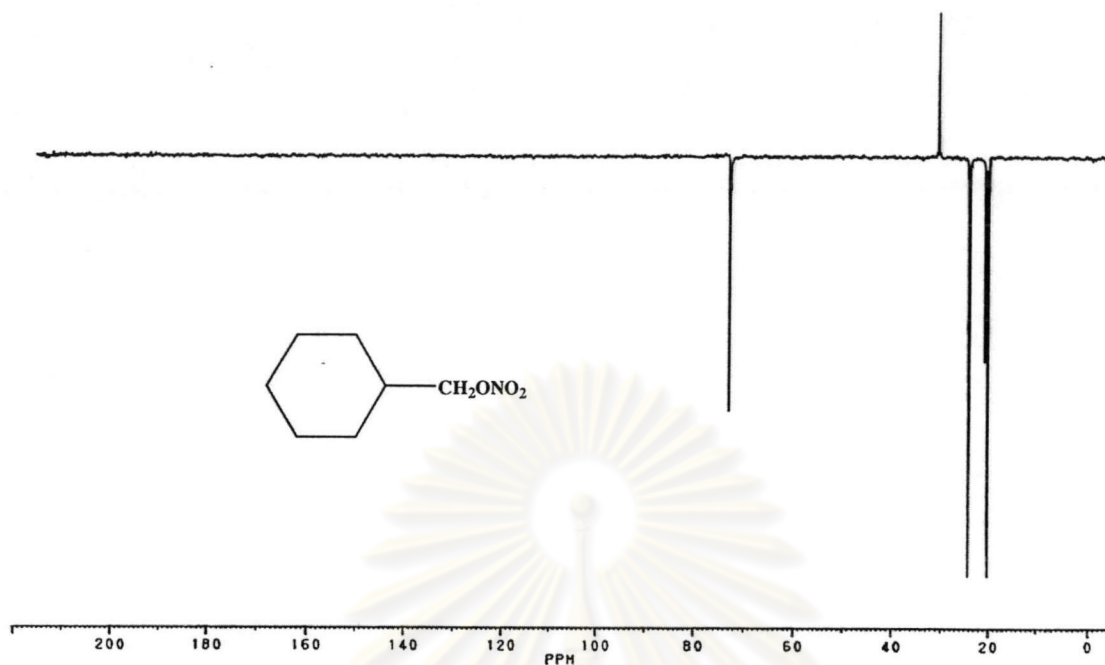


Figure A31 DEPT 135 Spectrum of Cyclohexylmethyl Nitrate (CDCl_3)

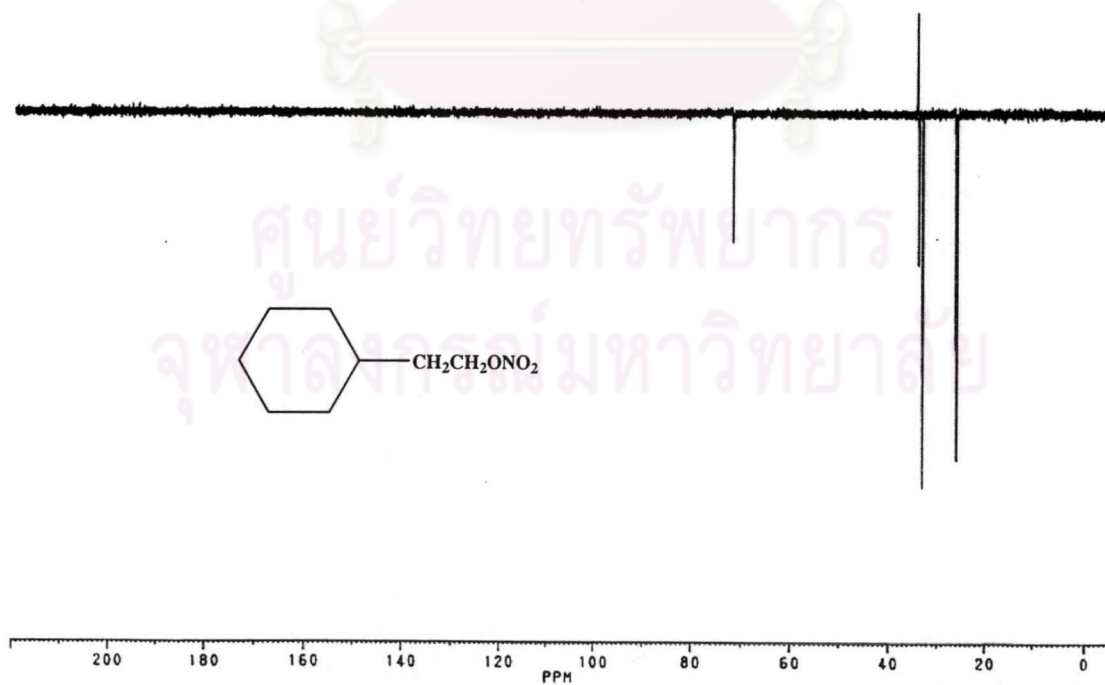


Figure A32 DEPT 135 Spectrum of 2-Cyclohexylethyl Nitrate (CDCl_3)

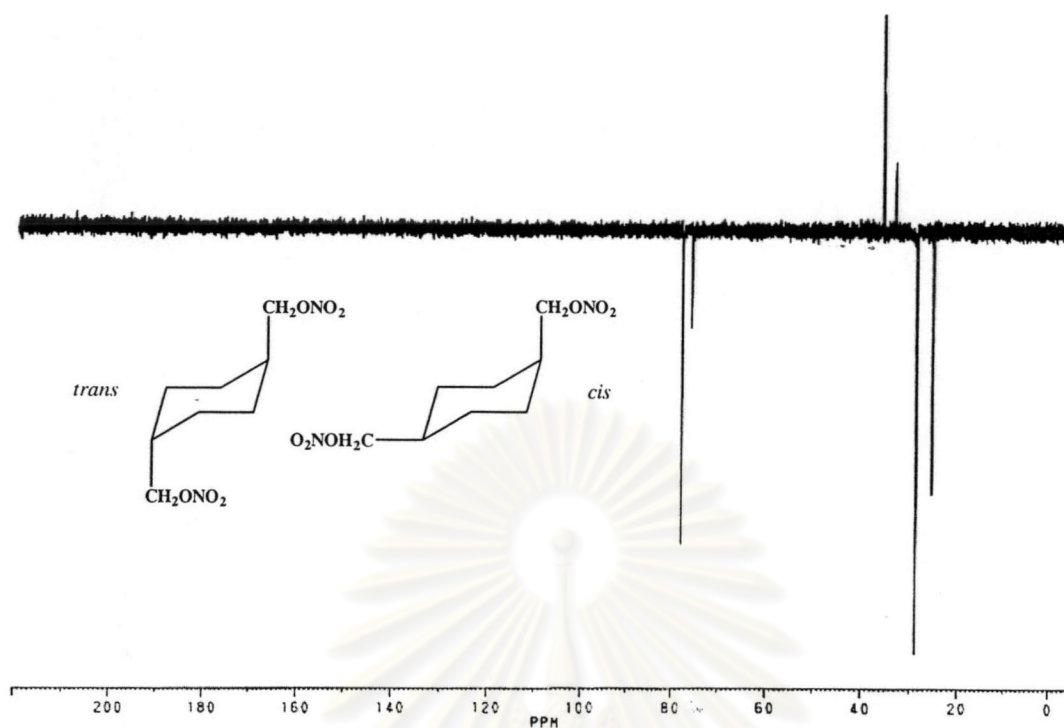


Figure A33 DEPT 135 Spectrum of 1,4-Cyclohexanedimethyl Nitrate (CDCl_3)

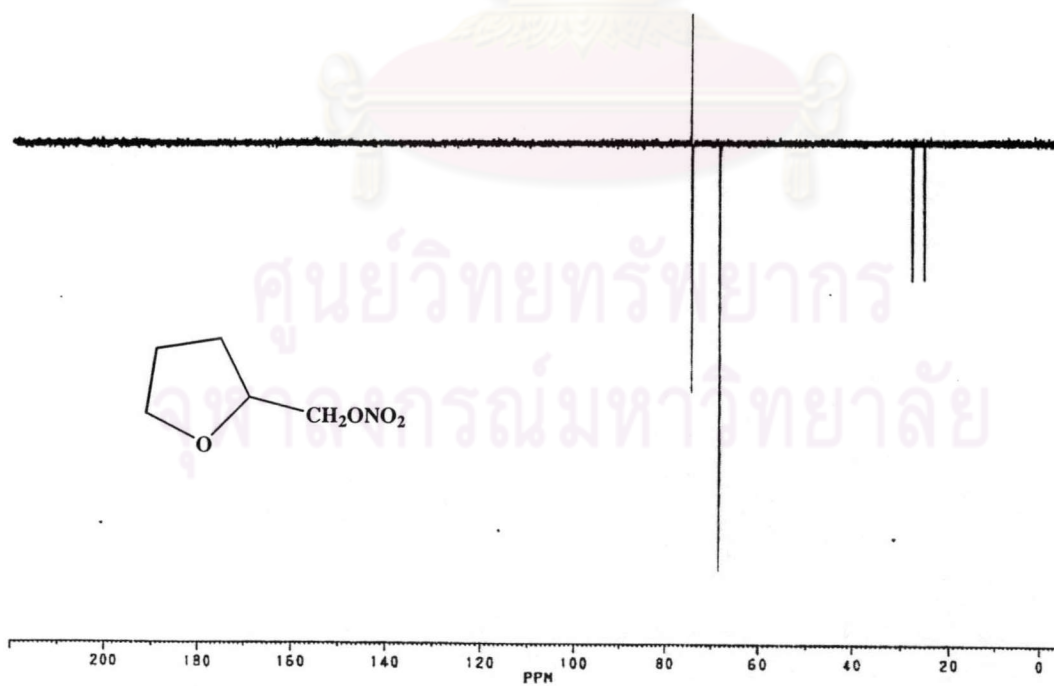


Figure A34 DEPT 135 Spectrum of Tetrahydrofurfuryl Nitrate (CDCl_3)

APPENDIX B

THE CALCULATION OF CETANE INDEX

The Calculated Cetane Index was determined from the following equation:

1. When it is not applicable to fuels containing additives for raising cetane number.

$$\begin{aligned} \text{Calculated Cetane Index} = & - 420.34 + 0.016G^2 + 0.192G \log M + 65.01(\log M)^2 \\ & - 0.0001809M^2 \dots\dots\dots(B1) \end{aligned}$$

2. When it is applicable to fuels containing additives for raising cetane number. The Calculated Cetane Index is determined from the equation B1 plus equation B2

$$\text{Improver Value} = 0.1742(0.1G)^{1.4444}(0.01M)^{1.0052} \{ \ln(1+17.5534) \} \dots\dots\dots(B2)$$

where

G = API gravity at 60°F, determined by Test Method ASTM D287 or D1298

M = Mid-boiling temperature, °F, determined by Test Method ASTM D 86 and corrected to standard barometric pressure.

D = Percent weight of cetane improver

For example:

Determine the cetane index of the blended diesel fuel with tetrahydrofurfuryl nitrate when percent weight of cetane improver at 0.10% wt., mid-boiling point at 525.2°F, API gravity = 38.0

Solution:

From the equation B1

$$\begin{aligned} \text{CCI} &= -420.34 + \{0.016 \times (38.0)^2\} + \{0.192(38.0) \times \log 525.2\} + \{65.01 \times (\log 525.2)^2\} \\ &\quad - \{0.0001809 \times (525.2)^2\} \\ &= 53.80 \end{aligned}$$

And from the equation B2

$$\begin{aligned} \text{Improver Value} &= 0.1742 \times (0.1 \times 38.0)^{1.4444} \times (0.01 \times 525.2)^{1.0052} \times \ln\{1 + (17.5534 \times 0.10)\} \\ &= 6.43 \end{aligned}$$

Therefore:

$$\begin{aligned} \text{CCI Improver} &= \text{CCI} + \text{Improver Value} \\ &= 53.80 + 6.43 \\ &= 60.23 \end{aligned}$$

APPENDEX C

THE CALCULATION OF CETANE NUBER

BY USING NOMOGRAPH

For example:

1. Predict the cetane number of the blended diesel fuel with fuel with tetrahydrofurfuryl nitrate when percent weight of cetane improver at 0.10%wt. and density at 15°C is 0.8344. The base cetane number is 54.0.
2. Identify the base fuel cetane number and density on the appropriate axes and draw a line joining these two points.
3. Connect the pivot point to the concentration and read back along the line to the predicted cetane number increase.
4. The increased cetane number is 5.00, so its cetane number is 59.00.



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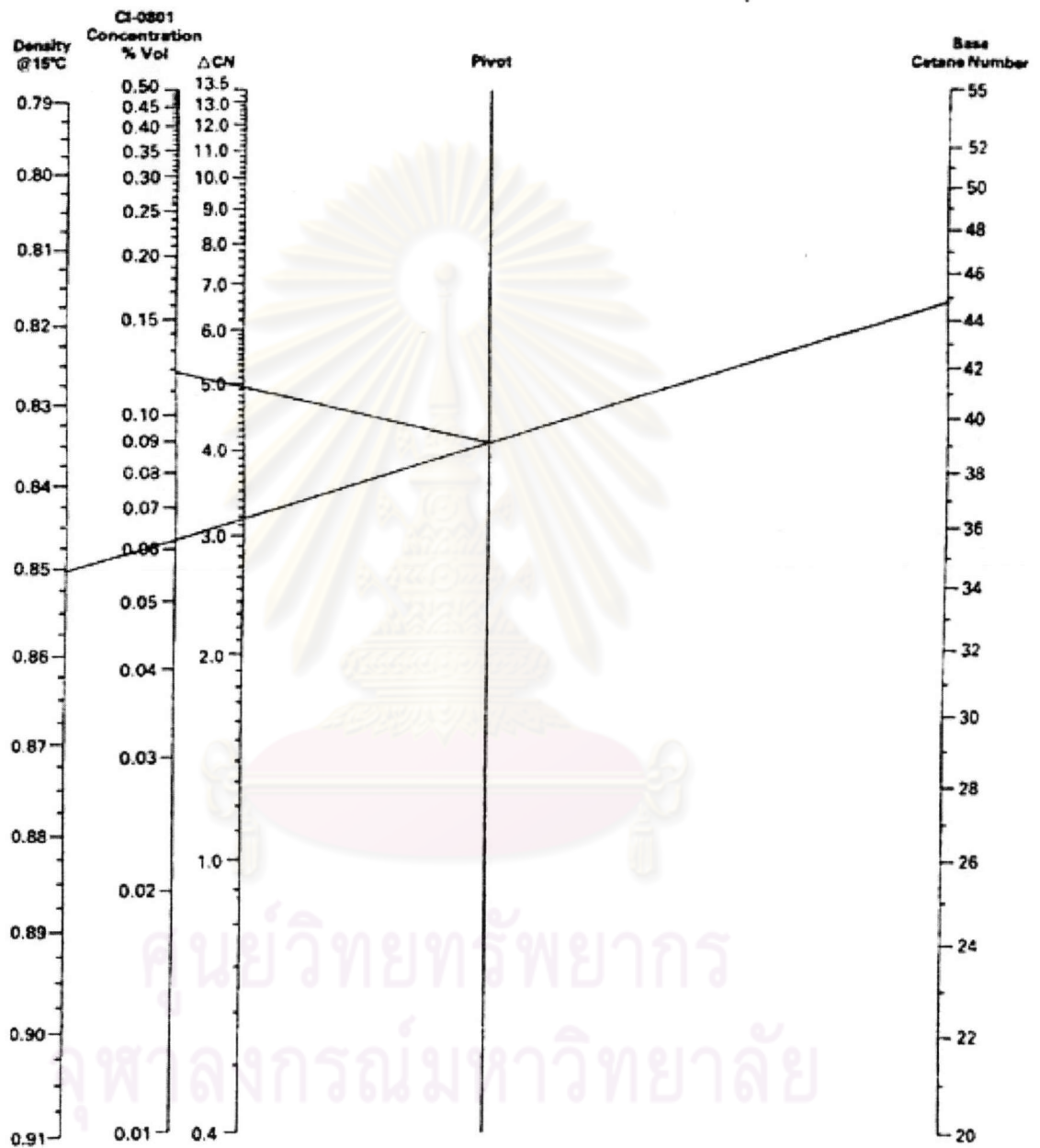


Figure C1 Example for the calculation of cetane number by using nomograph[10]

APPENDIX D

SPECIFICATION AND TEST METHOD FOR DIESEL

FUEL IN THAILAND

Characteristics	Specification		
	High-Speed Engine	Low-Speed Engine	Methods
Density at 15.6/15.6 °C	0.81-0.87	0.92	ASTM D1286
Cetane Number	min 47	min 45	ASTM D 613
Or Calculated Cetane Index	min 47	min 45	ASTM D 976
Viscosity at 40 °C, cSt	1.8-4.1	max 8.0	ASTM D 445
or at 50 °C, cSt		max 6.0	
Pour Point, °C	max 10	max 16	ASTM D 97
Sulfur Content, %wt.	max 0.25	max 1.5	ASTM D 129
Copper Strip Corrosion, number	max 1	-	ASTM D 130
Carbon Residue, %wt.	max 0.05	-	ASTM D 189
Water and Sediment, %vol.	max 0.05	max 0.3	ASTM D 2709
Ash Content, %wt.	max 0.01	max 0.02	ASTM D 482
Flash Point, °C	min 52	min 52	ASTM D 93
Distillation (temperature of 90% distillation)	max 357	-	ASTM D 86
Color	max 4.0	-	ASTM D 1500
Detergent Additive	Test by the Standard CUMMINS Tandem L-10 (Superior Level)	-	-

VITA

Theerawat Khankasikham was born on October 6, 1976 in Kamphaengphet, Thailand. He received his Bachelor's Degree of Science in Industrial Chemistry, Chiang Mai University in 1999. He continued his Master's Degree of Science in Petrochemistry and Polymer Science, Faculty of Science at Chulalongkorn University in 1999 and finished in 2002.



ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย