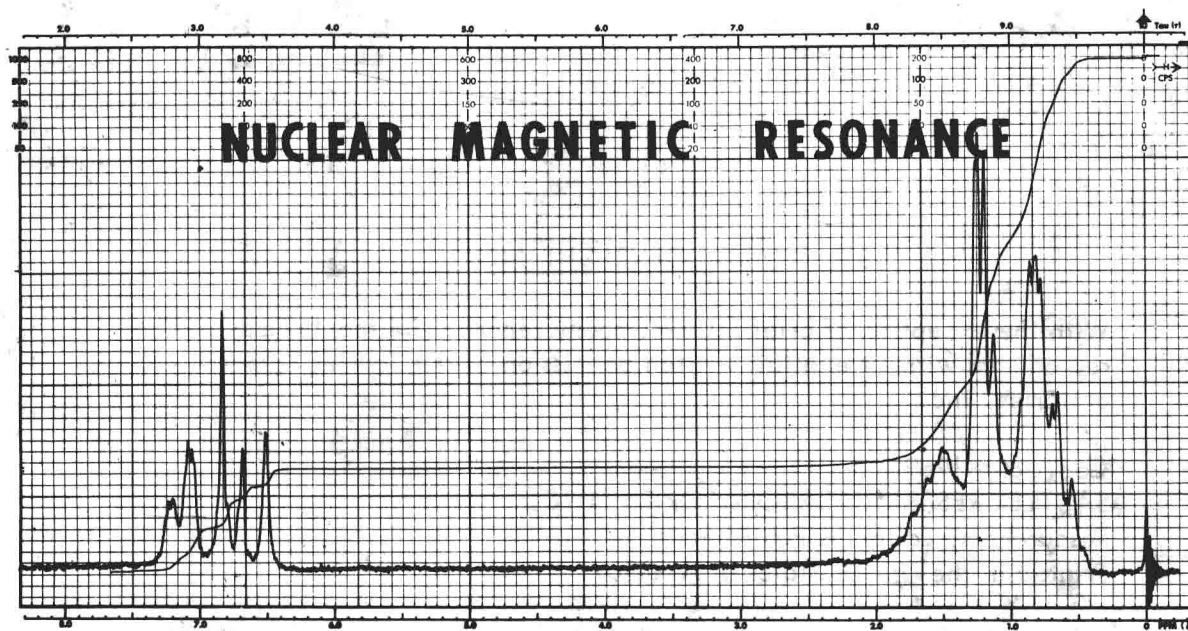




PLASTICIZERS 60 MHz SPECTRA

Vol. 1

E1M-E300M



LEGAL NOTICE

The publication of the physical data of the Sadtler Standard Spectra and the Sadtler Commercial Spectra is intended to be descriptive. As the samples of the materials represented have come generally from other sources than our own laboratories and frequently without the donors knowledge of their part in this publication, there can be no warranty either implied or otherwise.

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PLASTICIZERS

60 MHz NUCLEAR MAGNETIC RESONANCE SPECTRA

The Sadtler Commercial Collection of Plasticizers, 60 MHz Nuclear Magnetic Resonance Spectra, is an initial publication of 300 NMR spectra of commercially available plasticizers. The catalog contains representative spectra for almost every type of primary, secondary and specialty plasticizer listed in the "Plasticizer Chart", Modern Plastics Encyclopedia 1968.

Protons give rise to signals of varying position, intensity and complexity. The position of the signal, defined as the chemical shift, is dependent on the immediate electronic environment of the proton and is therefore an indication of its chemical nature. The intensity of a signal, which can be obtained by integration, is a measurement of the number of protons which cause that signal.

The integration curve for each spectrum is superimposed in color on the NMR scan.

INSTRUMENTATION

The spectra were determined at 60 mc/sec on a Varian Model A-60A spectrometer at magnet temperature of approximately 35°C (unless another temperature is noted on the spectrum). Each sample was dissolved in a suitable solvent together with tetramethylsilane (TMS) as an internal standard.

PRESENTATION

Each spectrum has an identifying NMR number, prefixed by **B** and suffixed by **M**; the corresponding IR number of the compound in the Sadtler Commercial Prism Collection is also shown.

The following information is also reported for each spectrum.

A. Product Data

1. Commercial name of product
2. Chemical description
3. Physical data (if known)
4. Source

B. Structural Assignment

If the structure of the compound is known, it has been drawn on the spectrum and proton assignments have been made. The assignment values are noted on the spectrum heading.

C. Instrument Data

1. Filter bandwidth
2. Sweep time
3. Sweep width
4. Sweep offset (if any)
5. Spectrum amplification
6. Integral amplification

Note: When more than one black curve is present on the graph (offset and/or amplification) the readings for this supplemental data are reported immediately after those for the original curve and are separated by a slash, e.g.: spectrum amplification 20/40, the first number would pertain to the original curve while the second would pertain to the amplified portion.

D. Solvent and Concentration

E. Pertinent Remarks

INDICES

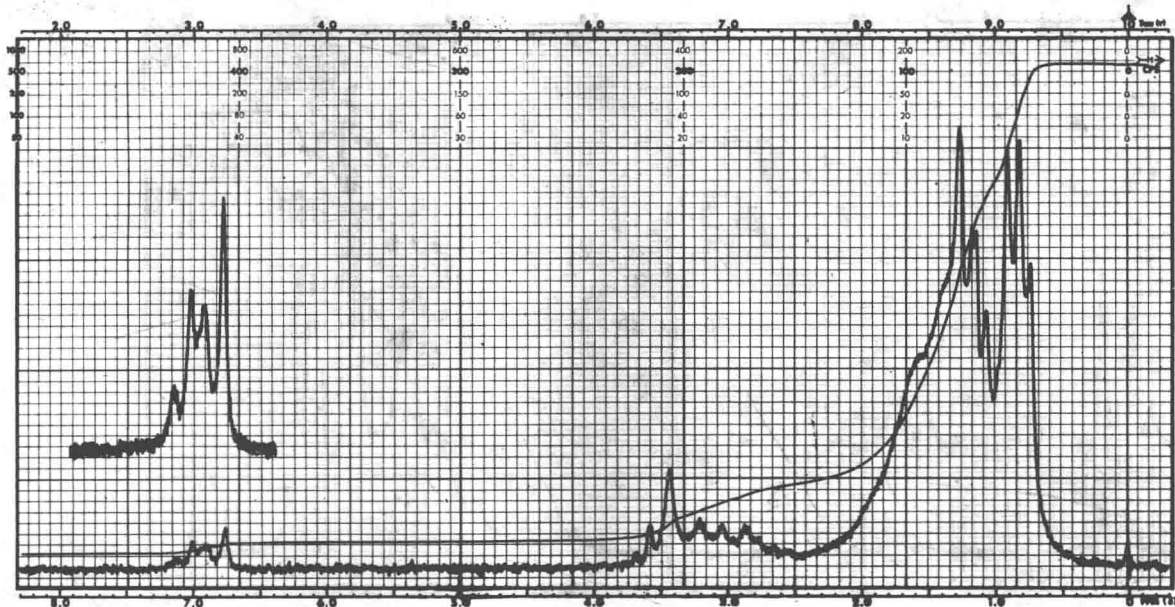
The indices furnished with this collection are as follows:

- Alphabetical Index according to commercial name and chemical name cross-references.
- Classification Index according to chemical type.
- Numerical Index according to NMR Spectrum number.
- Spec-Finder according to signal location and intensity.

The column of numbers entitled MFG CODE in the classification index refers to the code assigned to the manufacturer.

The three digit number in the column to the left of the compound name in the alphabetical index indicates the code assigned to the chemical class to which each product belongs. The infrared prism and grating spectrum numbers from the Sadtler Commercial Infrared Collection are also included in the indices. These codes will be useful to those using the other available spectra in conjunction with NMR. The titles and corresponding code numbers for the various types of plasticizers are listed below.

02	Abietic acid derivatives	44	Mellitic acid derivatives
04	Adipic acid derivatives	46	Myristic acid derivatives
06	Azelaic acid derivatives	50	Nitrile derivatives
08	Benzoic acid derivatives	52	Oleic acid derivatives
10	Biphenyl derivatives	54	Palmitic acid derivatives
12	Caprylic acid derivatives	56	Paraffins (Chlorinated)
14	Citric acid derivatives	58	Pelargonic acid derivatives
18	Epoxy derivatives	60	Pentaerythritol derivatives
20	Ether derivatives	61	Phenoxy derivatives
22	Ethylenediamine derivatives	62	Phosphoric acid derivatives
26	Formal derivatives	64	Phthalic acid derivatives
28	Fumaric acid derivatives	66	Polyesters
30	Glycerol derivatives	70	Ricinoleic acid derivatives
32	Glycol derivatives	72	Sebacic acid derivatives
34	Hydrocarbons	74	Stearic acid derivatives
36	Isobutyric acid derivatives	76	Styrene derivatives
38	Isophthalic acid derivatives	80	Sucrose derivatives
39	Lactams	82	Sulfonic acid derivatives
40	Lauric acid derivatives	99	Miscellaneous
42	Maleic acid derivatives		



E 1M

ABITOL

HYDROABIETYL ALCOHOL

E 2028

Sp. Gr. 20/20°C 1.007-1.008

n 20°C 1.528

A. V. 0.1-0.4

Source: Hercules, Inc.

ASSIGNMENTS

Filter bandwidth: 4
Sweep time: 250
Sweep width: 500
Sweep offset: -
Spectrum amp: 16
Integral amp: 80 (spec. amp. 0.8)
Solvent: CCl₄

Hz
sec
Hz
Hz

a _____ f _____
b _____ g _____
c _____ h _____
d _____ i _____
e _____ i _____

PLASTICIZERS

60 MHz N.M.R. © 1969

ABALYN

METHYL ABIETATE

E 2027

B. P. 360°C

Sp. Gr. 25°C 1.033

n 20°C 1.529

Flash Point 180°C

A. V. 6

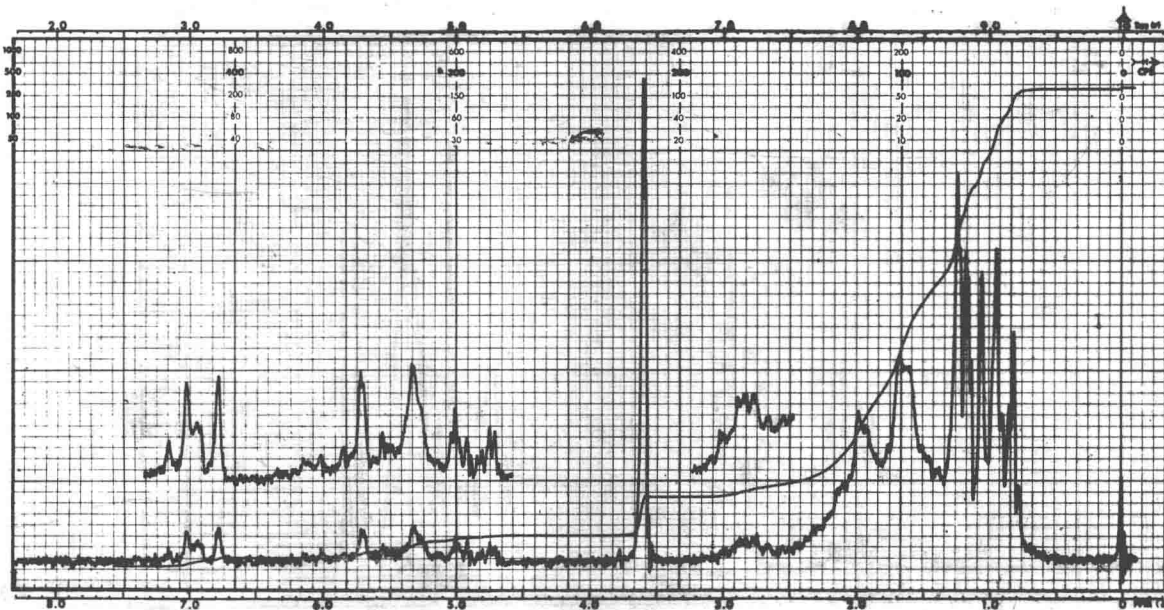
Source: Hercules, Inc.

ASSIGNMENTS

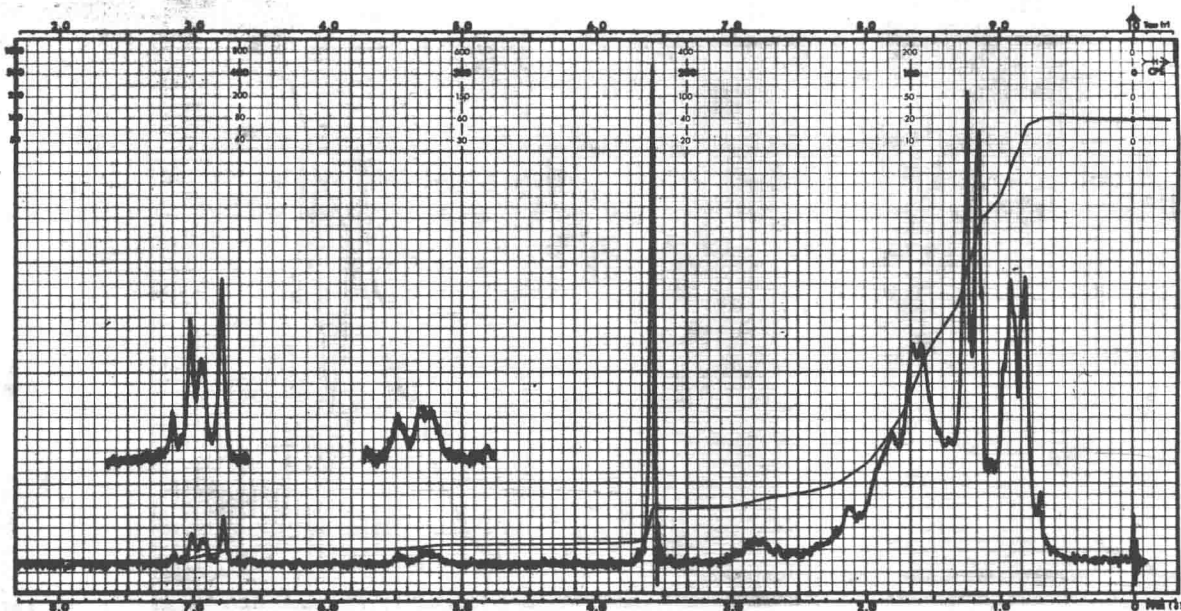
Filter bandwidth: 4
Sweep time: 250
Sweep width: 500
Sweep offset: -
Spectrum amp: 20/80
Integral amp: 80 (spec. amp. 1.6)
Solvent: CCl₄

Hz
sec
Hz
Hz

a _____ f _____
b _____ g _____
c _____ h _____
d _____ i _____
e _____ i _____



E 2M



E 3M

HERCOLYN

HYDROGENATED METHYL ABIETATE

E 2029

Sp. Gr. 25°C 1.026 n 20°C 1.518 A. V. 7
Source: Hercules, Inc.

Filter bandwidth: 4 Hz
Sweep time: 250/500 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 16/ 80
Integral amp: 80 (spec. amp. 8)
Solvent: CCl₄

ASSIGNMENTS

a	_____	f	_____
b	_____	g	_____
c	_____	h	_____
d	_____	i	_____
e	_____	i	_____

PLASTICIZERS

60 MHz N.M.R. © 1969

PALAMOLL 644 formerly PLASTICIZER ABG II

E 2406

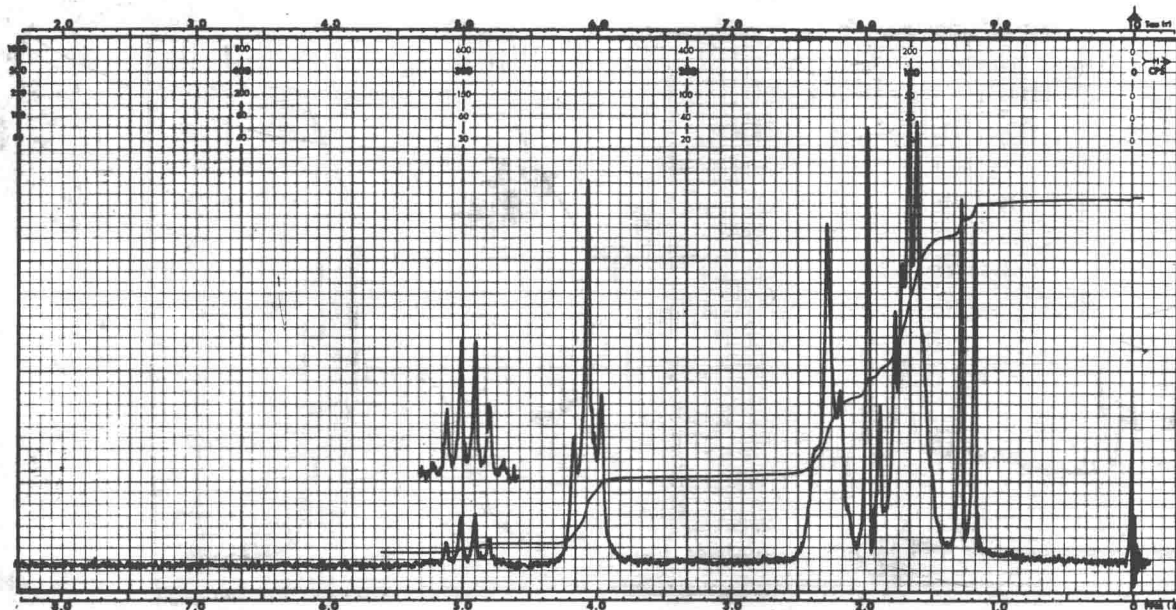
BUTYLENE GLYCOL POLYADIPATE

Sp. Gr. 20/4°C 1.13 n 20/D 1.47 Pour Point -14 to -19°C
Flash Point 175°C
Source: Badische Anilin- & Soda-Fabrik AG

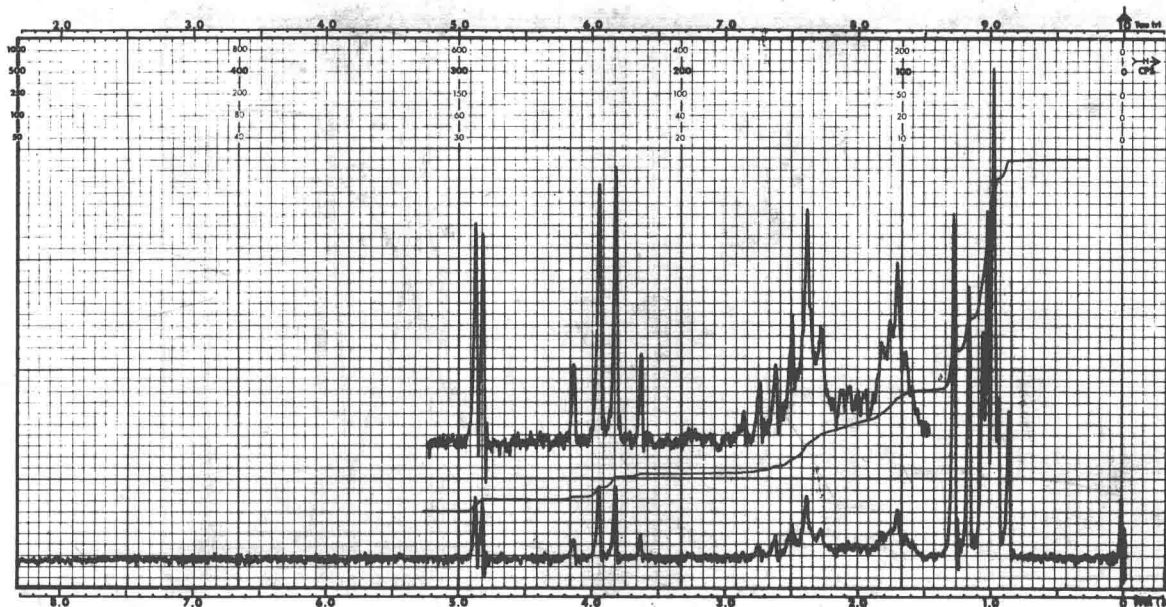
Filter bandwidth: 4 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 25
Integral amp: 80 (spec. amp. 1.6)
Solvent: CCl₄

ASSIGNMENTS

a	_____	f	_____
b	_____	g	_____
c	_____	h	_____
d	_____	i	_____
e	_____	i	_____



E 4M



E 5M

TEXANOL ADIPATE

E 2115

B. P. 331°C/760mm Sp. Gr. 20/20°C 1.00-1.01
Source: Eastman Chemical Products, Inc.

n_D 25/D 1.4528

ASSIGNMENTS

Filter bandwidth: 4/ 2 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 25/100
Integral amp: 80 (spec. amp. 4)
Solvent: CCl₄

a	_____	f	_____
b	_____	g	_____
c	_____	h	_____
d	_____	i	_____
e	_____	i	_____

PLASTICIZERS

60 MHz N.M.R. © 1969

HOWFLEX 3090

E 2467

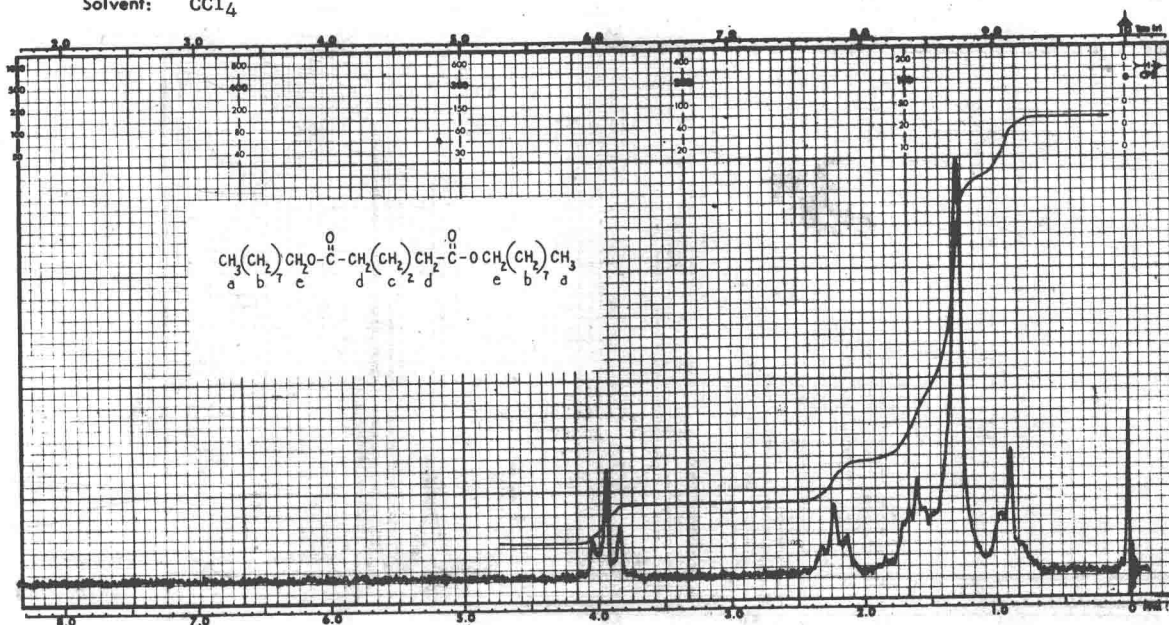
STRAIGHT CHAIN ALCOHOL ADIPATE

Source: Howards & Sons (Canada) Ltd.

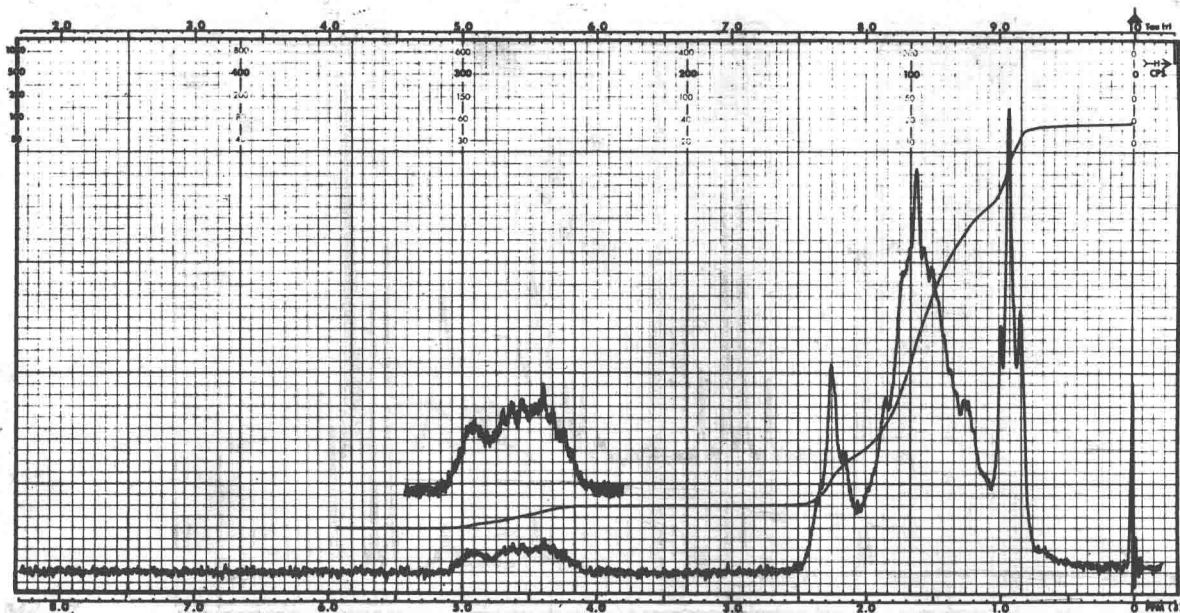
ASSIGNMENTS

Filter bandwidth: 4 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 10
Integral amp: 80 (spec. amp. 16)
Solvent: CCl₄

a	<u>0.91</u>	f	_____
b	<u>1.30</u>	g	_____
c	<u>1.61</u>	h	_____
d	<u>2.24</u>	i	_____
e	<u>3.93</u>	i	_____



E 6M



E 7M

SEXTOL ADIPATE

DI(METHYLCYCLOHEXYL) ADIPATE

E 2575

B. P. 190-200°C/3mm Sp. Gr. 25°C 1.007

M. W. 338

n 25°C 1.468

Flash Point 190°C

Source: Howards & Sons (Canada) Ltd.

ASSIGNMENTS

Filter bandwidth: 4 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 40
Integral amp: 80 (spec. amp. 2)
Solvent: CDC₁₃

a	_____	f	_____
b	_____	g	_____
c	_____	h	_____
d	_____	i	_____
e	_____	i	_____

PLASTICIZERS

60 MHz N.M.R. © 1969

E 2888

DIETHYL ADIPATE

B. P. 239-241°C/761mm (lit.)

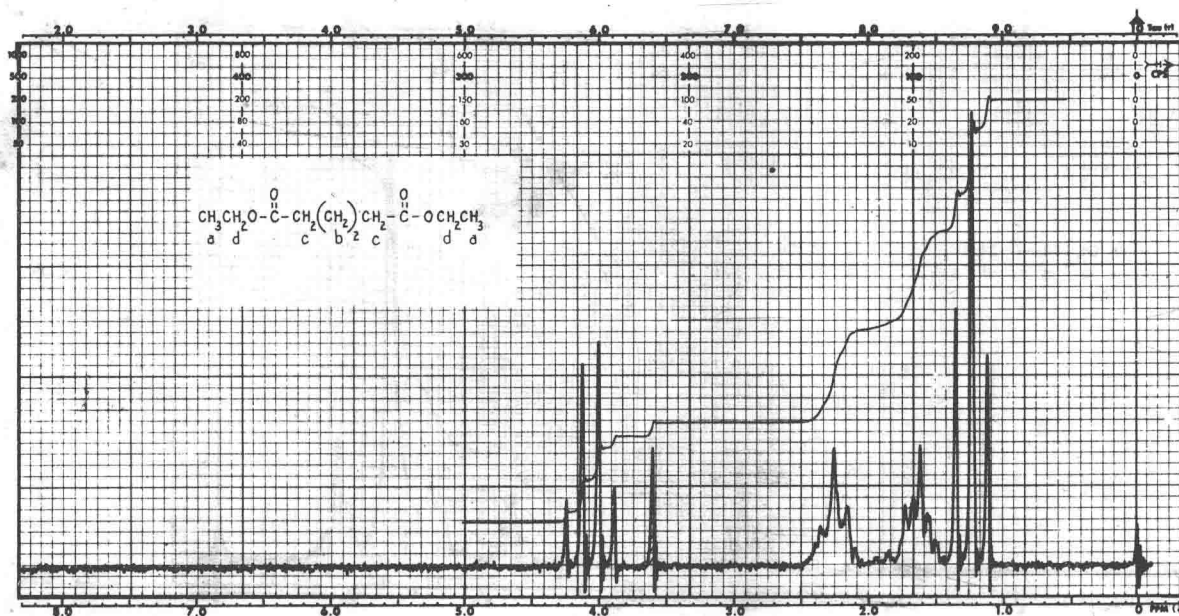
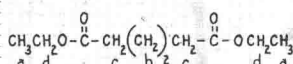
M. W. 202.25

Source: W. R. Grace & Co., Hatco Chemical Div.

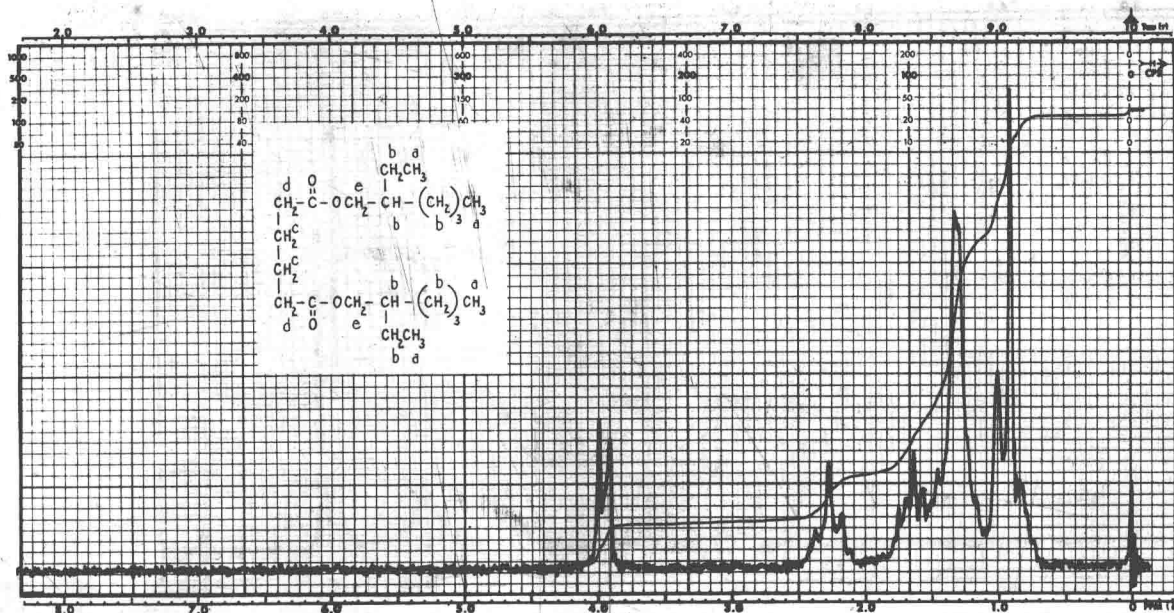
ASSIGNMENTS

Filter bandwidth: 4 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 10
Integral amp: 80 (spec. amp. 1.25)
Solvent: CCl₄

a	1.24	f	_____
b	1.63	g	_____
c	2.27	h	_____
d	4.07	i	_____
e	3.61 imp.	i	_____



E 8M



E 9M

NUOPLAZ 6815 formerly LEFLEX 6815

E 2409

DI(2-ETHYLHEXYL) ADIPATE

B. P. 214°C/5mm n 20°C 1.446-1.447

Flash Point (COC) 385°F

Source: Tenneco Chemicals, Inc., Nuodex Div.

ASSIGNMENTS

Filter bandwidth: 4 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 16
Integral amp: 80 (spec. amp. 2)
Solvent: CCl₄

a 0.91 f
b 1.10-1.60 g
c 1.63 h
d 2.28 i
e 3.96 i

PLASTICIZERS

60 MHz N.M.R. © 1969

ADIMOLL DB

DIBUTYL ADIPATE

E 2103

B. P. 168-170°C/17mm Sp. Gr. 25°C 0.961

n 25°C 1.434 Flash Point 116°C

Source: Farbenfabriken Bayer AG

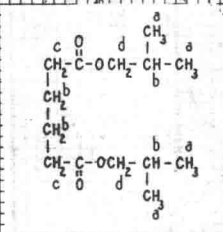
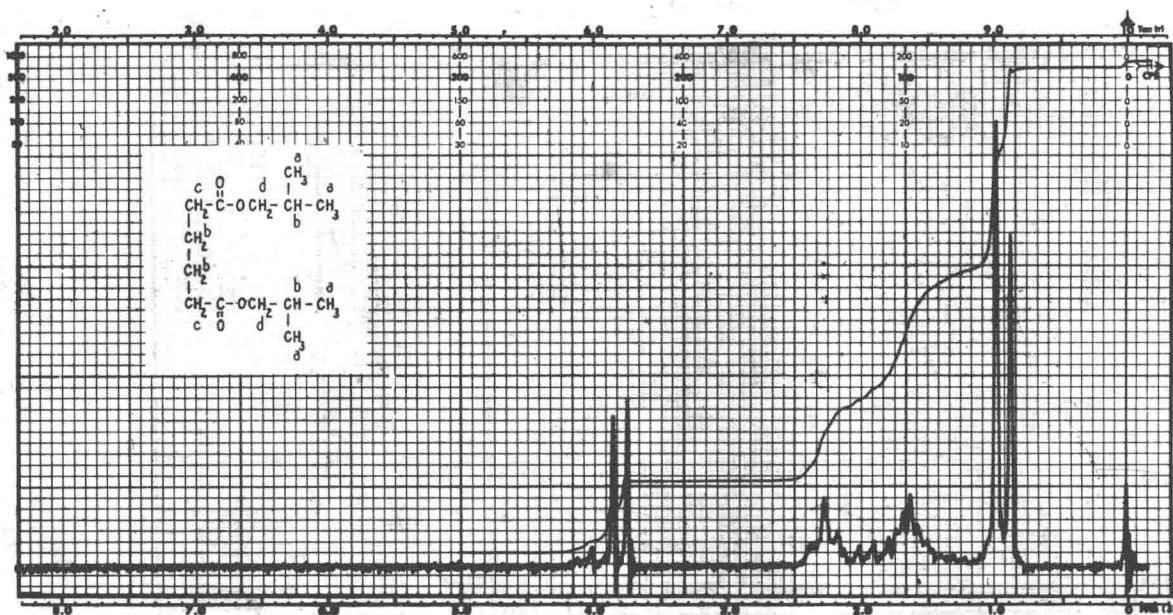
ASSIGNMENTS

Filter bandwidth: 4 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 32
Integral amp: 80 (spec. amp. 3.2)
Solvent: CCl₄

a 0.95 f
b 1.10-2.00 g
c 2.26 h
d 4.01 i
e



E 10M



E 11M

HATCOL DIBA

E 2462

DIISOBUTYL ADIPATE

Source: W. R. Grace & Co., Hatco Chemical Div.

ASSIGNMENTS

Filter bandwidth: 4 Hz
 Sweep time: 250 sec
 Sweep width: 500 Hz
 Sweep offset: - Hz
 Spectrum amp: 8
 Integral amp: 80 (spec. amp. 2.5)
 Solvent: CCl₄

a	<u>0.94</u>	f	<u> </u>
b	<u>1.30-2.10</u>	g	<u> </u>
c	<u>2.29</u>	h	<u> </u>
d	<u>3.81</u>	i	<u> </u>
e	<u> </u>	j	<u> </u>

PLASTICIZERS

60 MHz N.M.R. © 1969

E 2669

ADIPOL DIBA

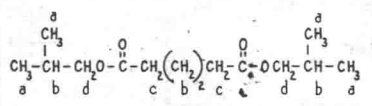
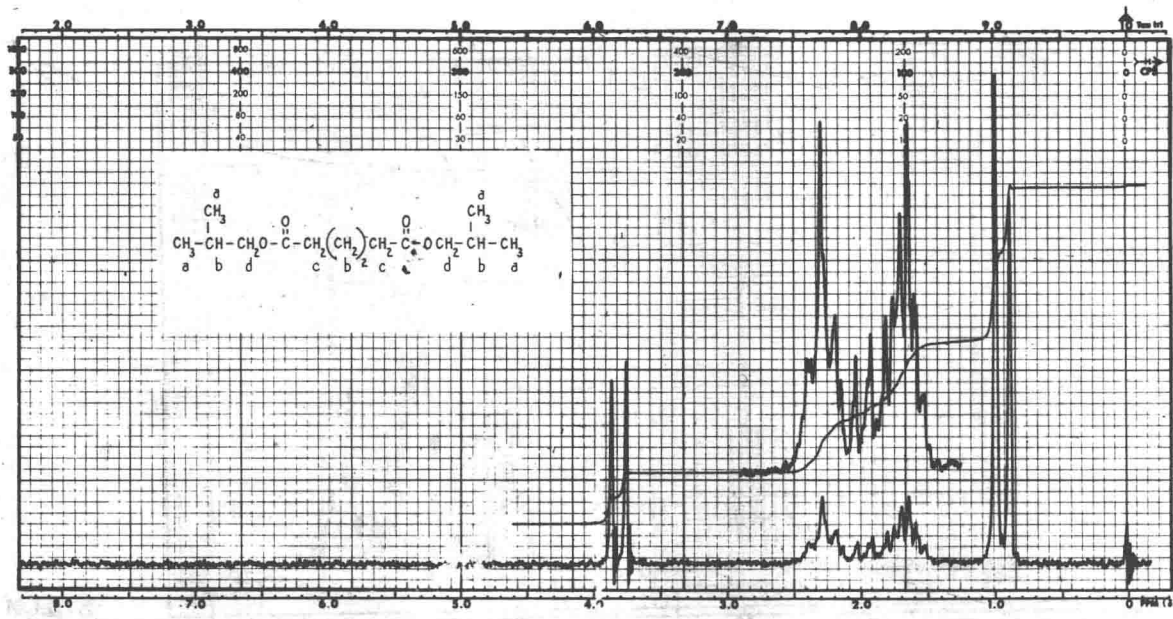
DIISOBUTYL ADIPATE

Source: FMC Corp., Organic Chemicals Div.

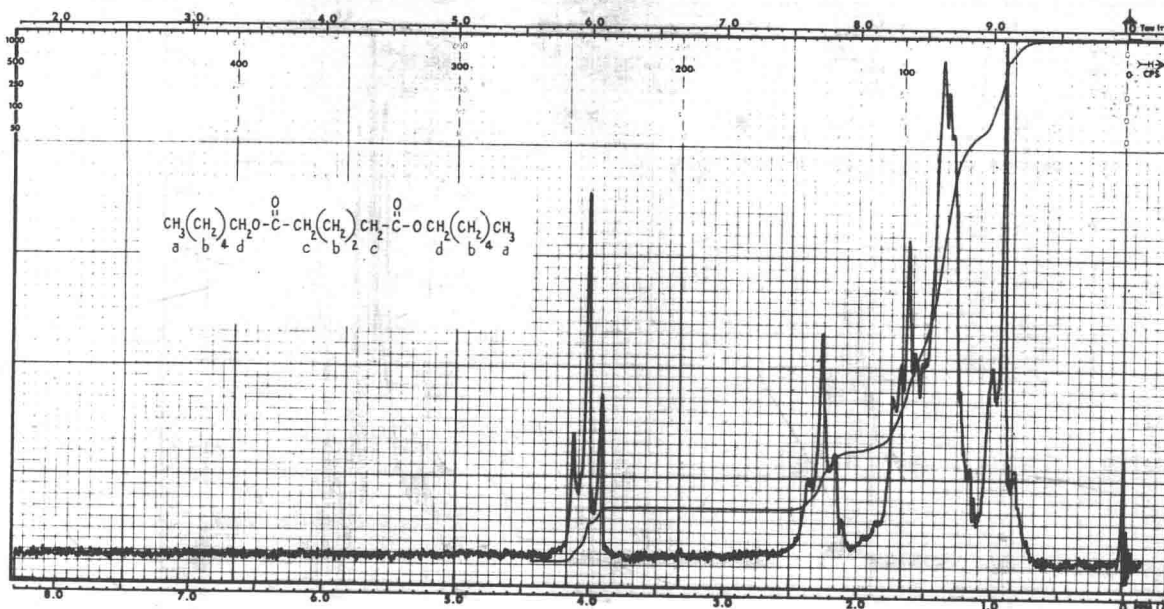
ASSIGNMENTS

Filter bandwidth: 4 Hz
 Sweep time: 250/500 sec
 Sweep width: 500 Hz
 Sweep offset: - Hz
 Spectrum amp: 6.3/ 40
 Integral amp: 80 (spec. amp. 1.6)
 Solvent: CCl₄

a	<u>0.95</u>	f	<u> </u>
b	<u>1.47-2.17</u>	g	<u> </u>
c	<u>2.29</u>	h	<u> </u>
d	<u>3.81</u>	i	<u> </u>
e	<u> </u>	j	<u> </u>



E 12M



E 13M

KESSCOFLEX DHA

E 2865

DIHEXYL ADIPATE

Source: Kessler Chemical Co.

Filter bandwidth: 4 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 25
Integral amp: 80 (spec. amp. 2)
Solvent: CCl_4

ASSIGNMENTS

a	0.92	f	
b	1.11-1.91	g	
c	2.28	h	
d	4.00	i	
e		i	

PLASTICIZERS

60 MHz N.M.R. © 1969

TRUFLEX DOA

DI(2-ETHYLHEXYL) ADIPATE

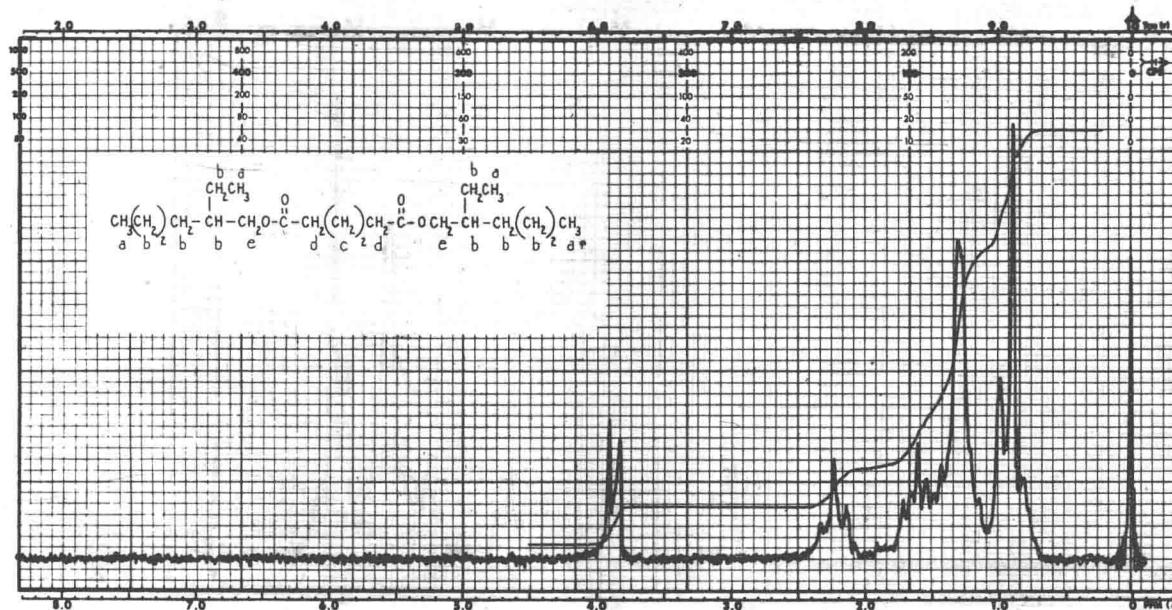
E 2455

Sp. Gr. 25°C 0.927 Visc. 20 cps A. V. 0.05
Source: Thompson Apex Co.

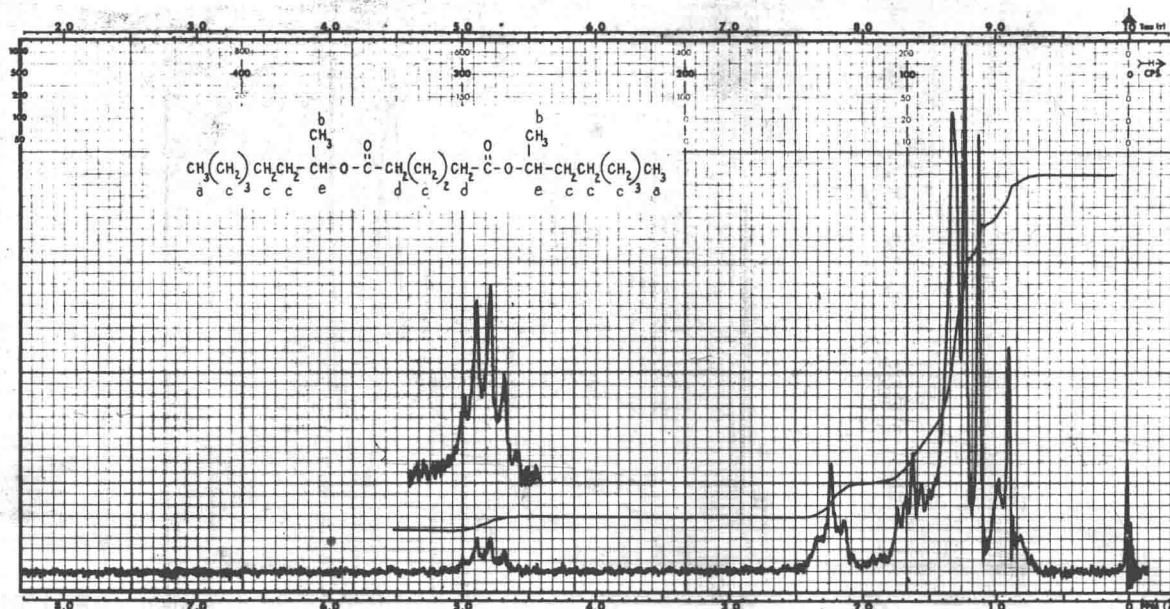
Filter bandwidth: 4 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 16
Integral amp: 80 (spec. amp. 2)
Solvent: CCl_4

ASSIGNMENTS

a	0.91	f	
b	1.10-1.55	g	
c	1.60	h	
d	2.23	i	
e	3.88	i	



E 14M



E 15M

DICAPRYL ADIPATE

E 2233

B. P. 213-217°C/4mm Sp. Gr. 20°C 0.9135
Source: W. R. Grace & Co., Hatco Chemical Div.

Filter bandwidth: 4/ 2 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 25/160
Integral amp: 80 (spec. amp. 2.5)
Solvent: CCl₄

ASSIGNMENTS

a	0.91	f	
b	1.19	g	
c	1.19-1.81	h	
d	2.24	i	
e	4.83	j	

PLASTICIZERS

60 MHz N.M.R. © 1969

SHAWINIGAN DOA

DIOCTYL ADIPATE

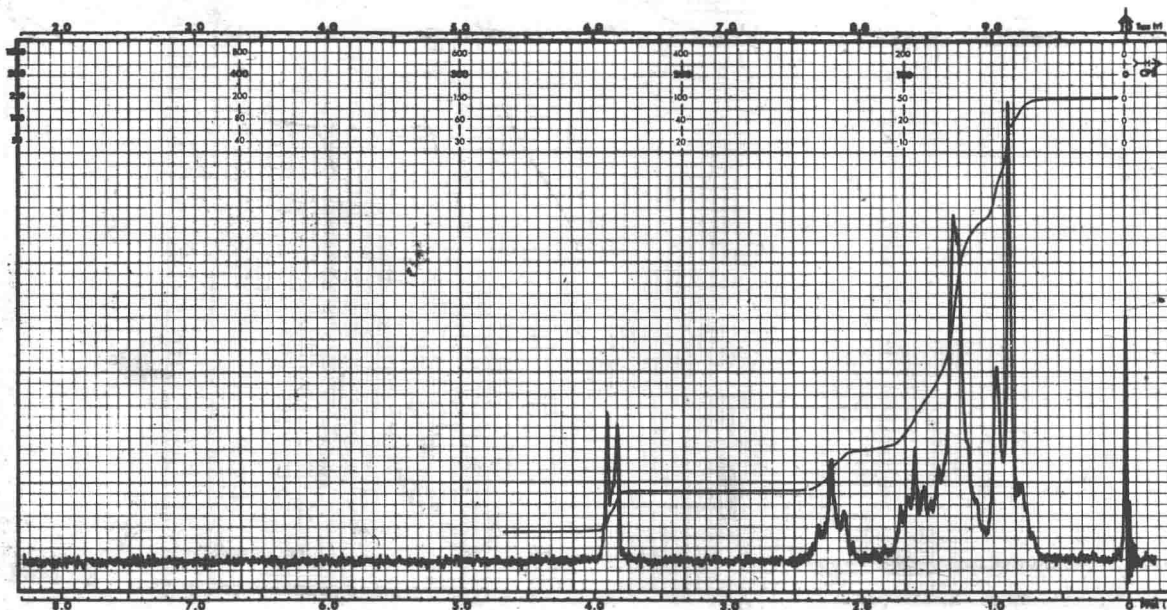
E 2489

M. P. < -60°C Mid - B. P. 214°C/5mm Sp. Gr. 20/20°C 0.928
Visc. 25°C 11 cps Flash Point (OC) 381°F
Source: Shawinigan Chemicals Ltd.

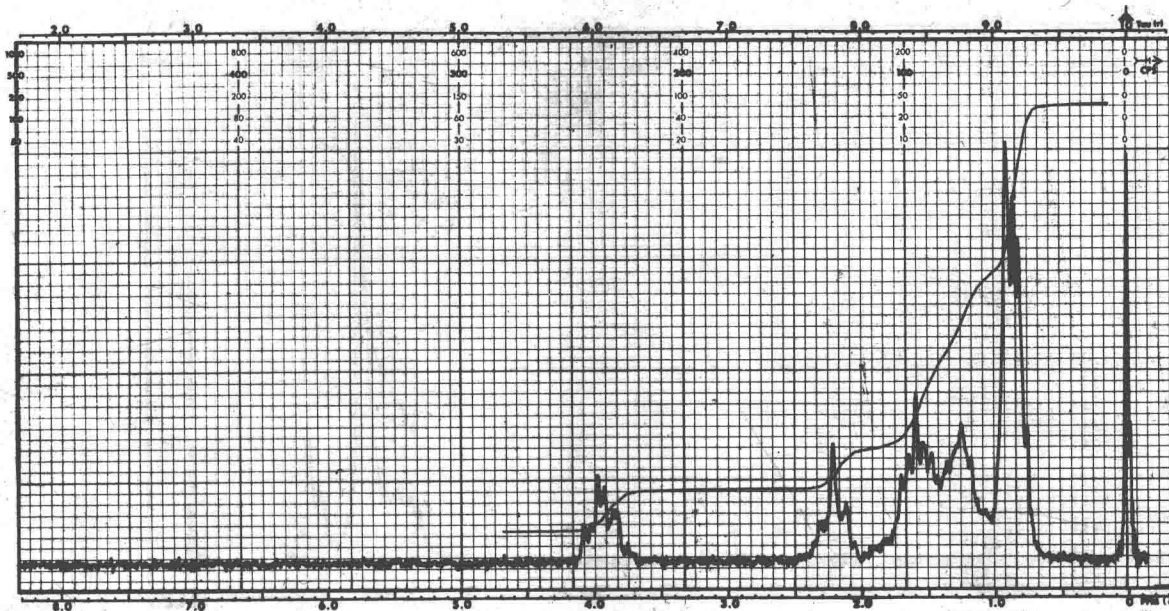
Filter bandwidth: 4 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 12.5
Integral amp: 80 (spec. amp. 1.6)
Solvent: CCl₄

ASSIGNMENTS

a		f	
b		g	
c		h	
d		i	
e		j	



E 16M



E 17M

HOWFLEX DIOA

DIISOCTYL ADIPATE

E 2477

Source: Howards & Sons. (Canada) Ltd.

Filter bandwidth: 4 Hz
 Sweep time: 250 sec
 Sweep width: 500 Hz
 Sweep offset: - Hz
 Spectrum amp: 20
 Integral amp: 80 (spec. amp. 2)
 Solvent: CCl_4

ASSIGNMENTS

a	_____	f	_____
b	_____	g	_____
c	_____	h	_____
d	_____	i	_____
e	_____	i	_____

PLASTICIZERS

60 MHz N.M.R. © 1969

NUOPLAZ 6810 formerly LEFLEX 6810

OCTYL DECYL ADIPATE

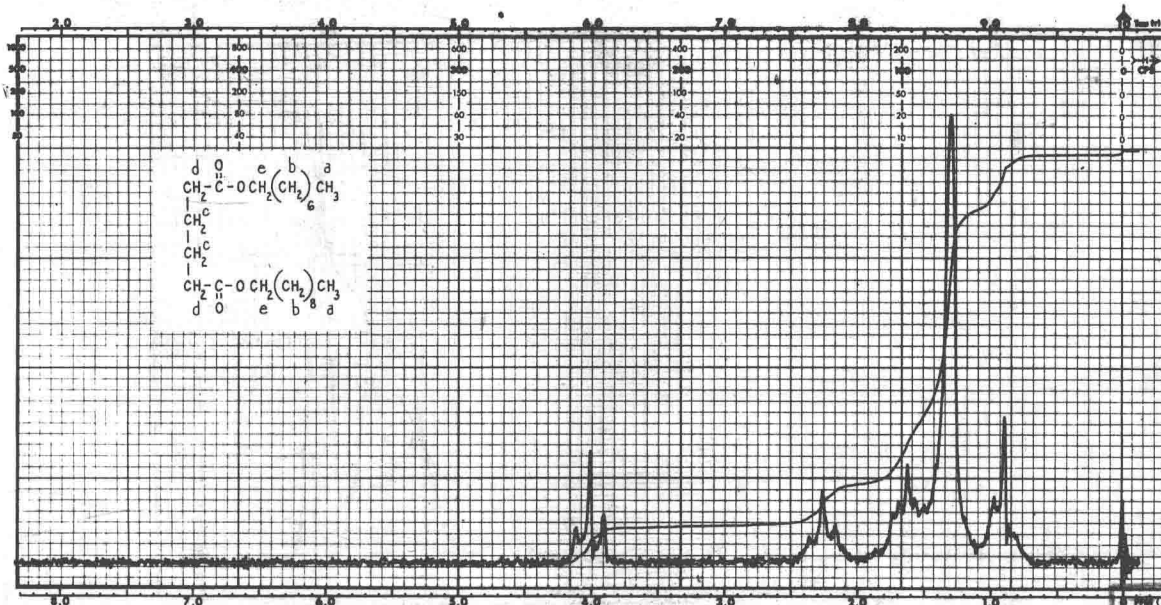
E 2408

B. P. 210-235°C/5mm Sp. Gr. 25°C 0.915-0.924
 n 25°C 1.447-1.451 Flash Point (COC) 200-235°F
 Source: Tenneco Chemicals, Inc., Nuodex Div.

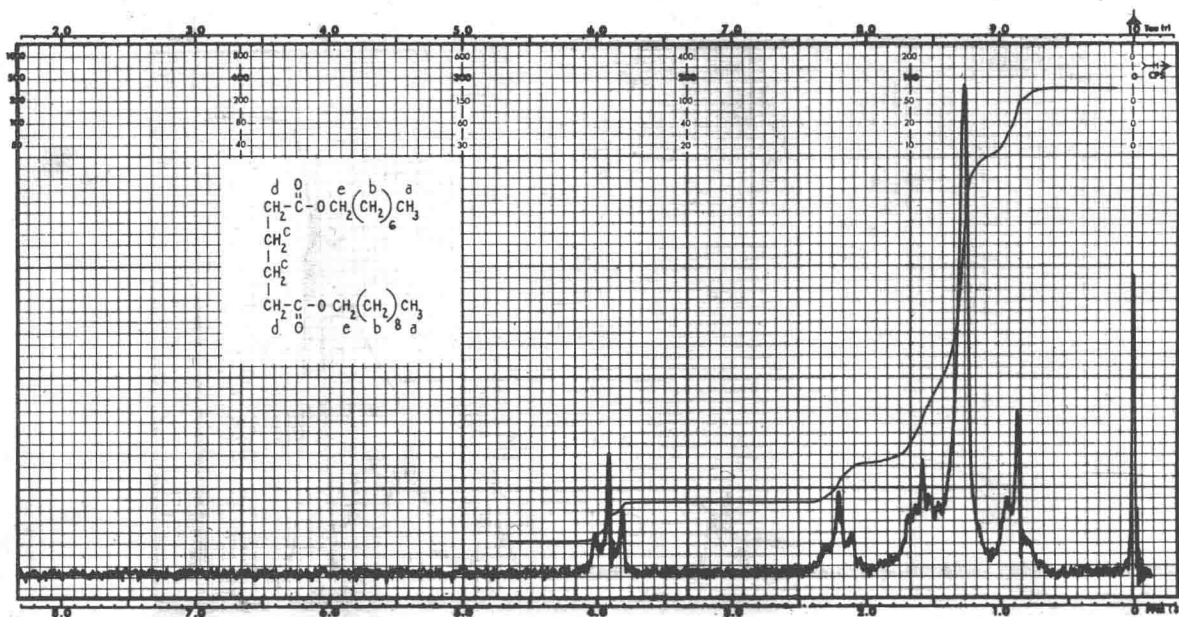
Filter bandwidth: 4 Hz
 Sweep time: 250 sec
 Sweep width: 500 Hz
 Sweep offset: - Hz
 Spectrum amp: 12.5
 Integral amp: 80 (spec. amp. 2)
 Solvent: CCl_4

ASSIGNMENTS

a	<u>0.90</u>	f	_____
b	<u>1.10-1.60</u>	g	_____
c	<u>1.61</u>	h	_____
d	<u>2.28</u>	i	_____
e	<u>4.01</u>	i	_____



E 18M



E 19M

TRUFLEX 200

n-OCTYL n-DECYL ADIPATE

E 2452

Sp. Gr. 0.915

Visc. 20 cps

A. V. 0.05

Source: Thompson Apex Co.

ASSIGNMENTS

Filter bandwidth: 4 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 16
Integral amp: 80 (spec. amp. 2.5)
Solvent: CCl₄

a 0.89 f
b ca 1.27 g
c 1.58 h
d 2.21 i
e 3.91 i

PLASTICIZERS

60 MHz N.M.R. © 1969

RUCOFLEX ODA

ISOOCYL ISODECYL ADIPATE

E 2416

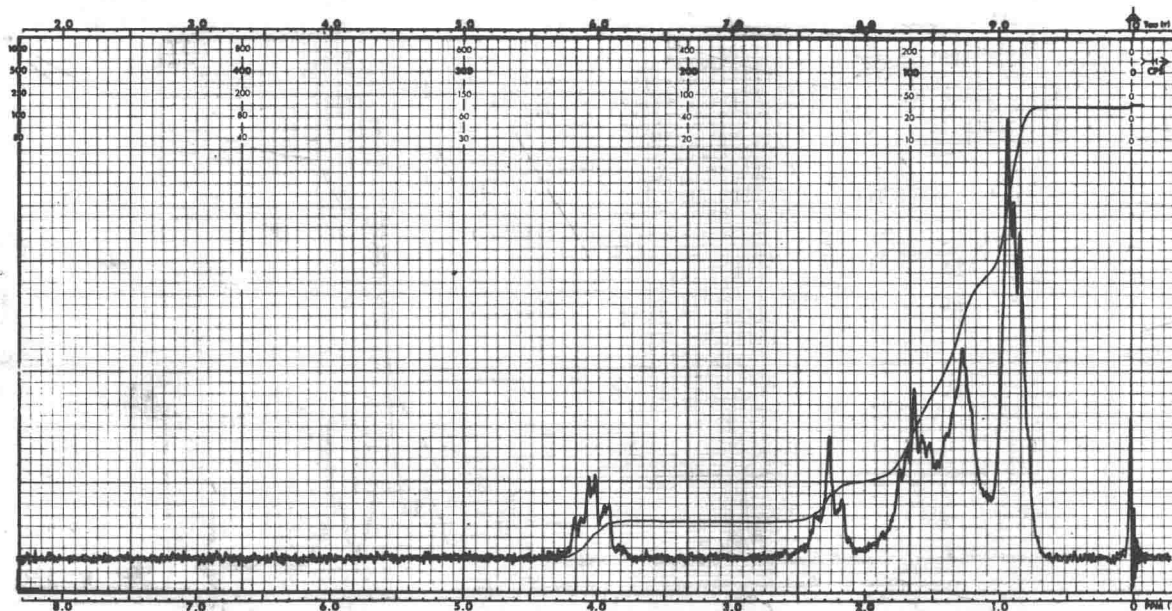
Distillation Range 5-95% 222-241°C/5mm
n 23°C 1.4487 Flash Point 405°F
Source: Hooker Chemical Corp., Ruco Div.

Sp. Gr. 20/20°C 0.921-0.927
S. V. 280

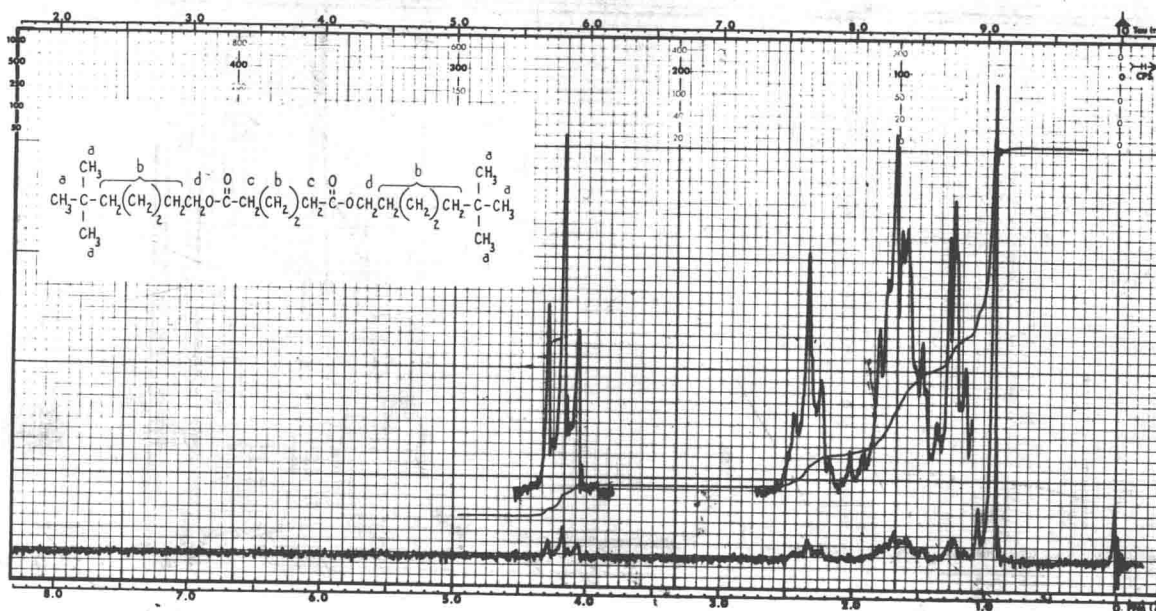
ASSIGNMENTS

Filter bandwidth: 4 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 25
Integral amp: 80 (spec. amp. 2.5)
Solvent: CCl₄

a f
b g
c h
d i
e i



E 20M



E 21M

DINONYL ADIPATE

DI (TRIMETHYLHEXYL) ADIPATE

E 2518

Sp. Gr. 25°C 0.915

M. W. 398.6

Flash Point 295°F

Source: Pittsburgh Chemical Co.

ASSIGNMENTS

Filter bandwidth: 4
Sweep time: 250
Sweep width: 500
Sweep offset: -
Spectrum amp: 3.2/40
Integral amp: 80 (spec. amp. 1.6)
Solvent: CCl₄

Hz
sec
Hz
Hz

a	<u>0.95</u>	f	<u> </u>
b	<u>1.02-2.11</u>	g	<u> </u>
c	<u>2.34</u>	h	<u> </u>
d	<u>4.17</u>	i	<u> </u>
e	<u> </u>	i	<u> </u>

PLASTICIZERS

60 MHz N.M.R. © 1969

NUOPLAZ 6817 formerly LEFLEX 6817

DIDECYL ADIPATE

E 2411

B. P. 349°C/760mm

Sp. Gr. 20°C 0.917-0.922

n 25°C 1.4495-1.4510

Flash Point (COC) 425°F

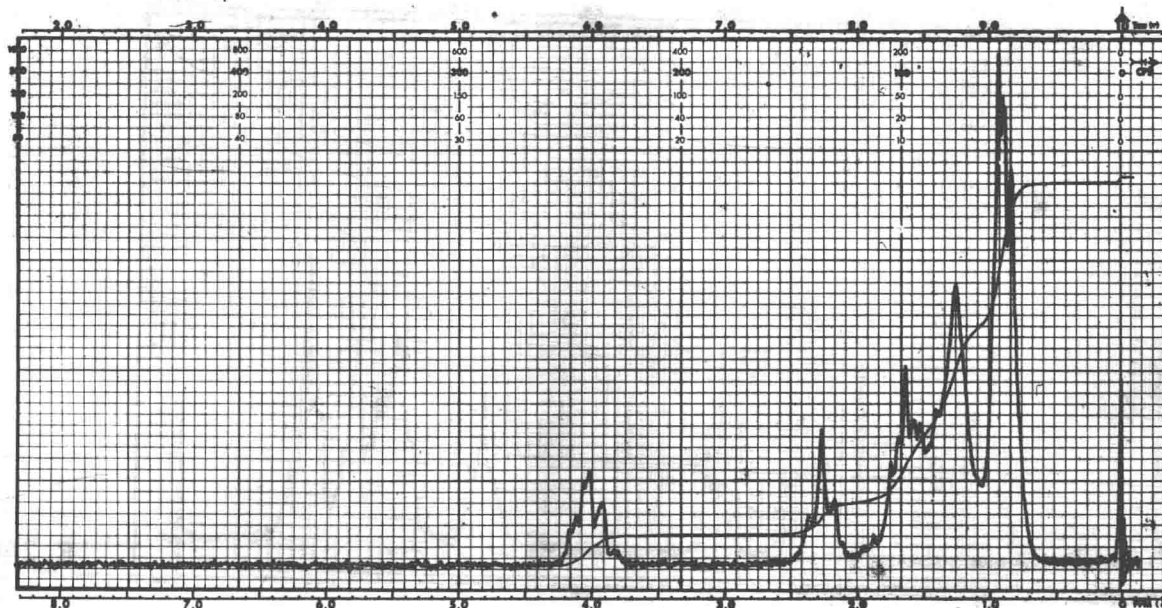
Source: Tenneco Chemicals, Inc., Nuodex Div.

ASSIGNMENTS

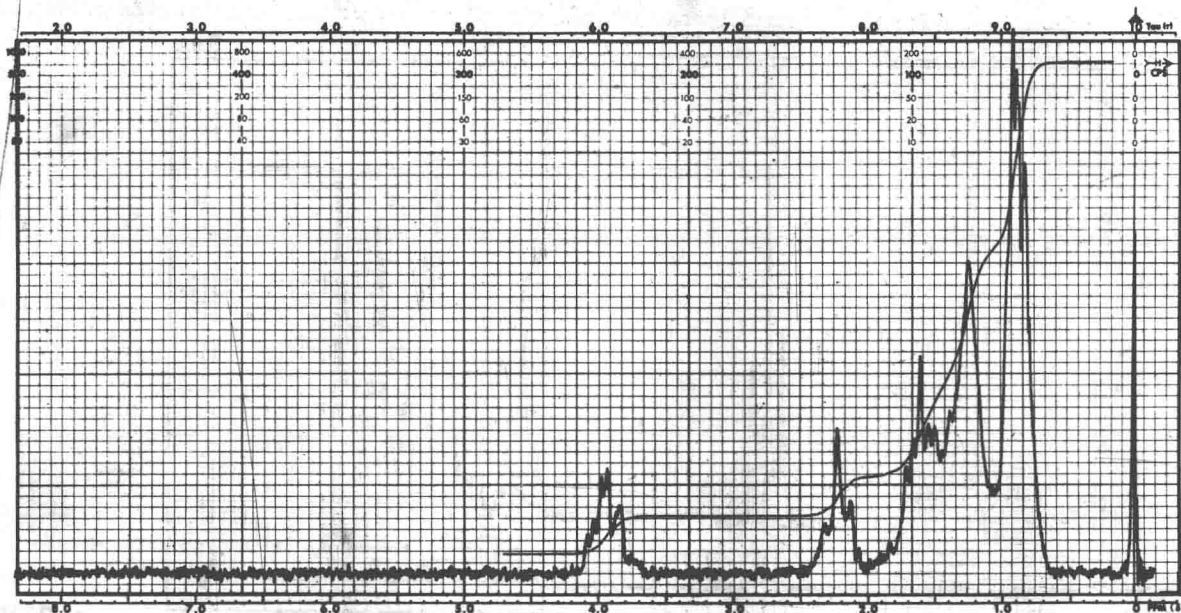
Filter bandwidth: 4
Sweep time: 250
Sweep width: 500
Sweep offset: -
Spectrum amp: 40
Integral amp: 80 (spec. amp. 2.5)
Solvent: CCl₄

Hz
sec
Hz
Hz

a	<u> </u>	f	<u> </u>
b	<u> </u>	g	<u> </u>
c	<u> </u>	h	<u> </u>
d	<u> </u>	i	<u> </u>
e	<u> </u>	i	<u> </u>



E 22M



E 23M

HARFLEX 212

DIISODECYL ADIPATE

E 2495

M. P. -70°C B. P. 239-248°C/4mm Sp. Gr. 20/20°C 0.915-0.921

Visc. 25°C 23 cps Flash Point 444°F Fire Point 500°F

Source: Wallace & Tiernan, Inc., Harchem Div.

Filter bandwidth: 4 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 32
Integral amp: 80 (spec. amp. 2.5)
Solvent: CCl₄

ASSIGNMENTS
a _____ f _____
b _____ g _____
c _____ h _____
d _____ i _____
e _____

PLASTICIZERS

60 MHz N.M.R. © 1969

E 2335

ADIMOLL BB

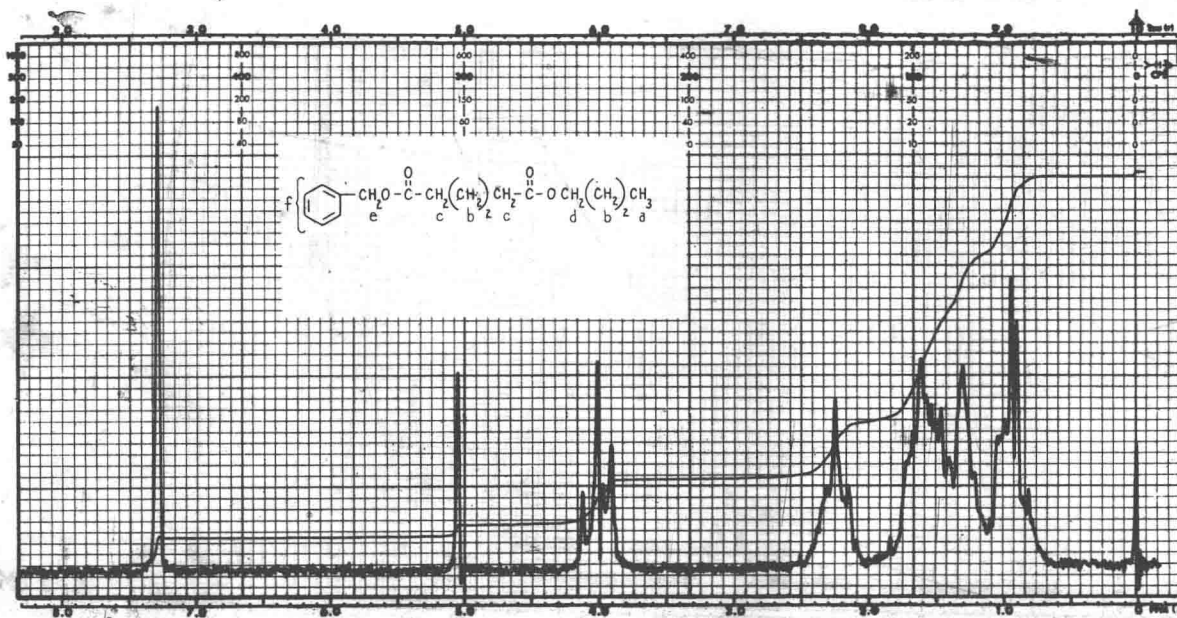
BENZYL n-BUTYL ADIPATE

Source: Farbenfabriken Bayer AG

Filter bandwidth: 4 Hz
Sweep time: 250 sec
Sweep width: 500 Hz
Sweep offset: - Hz
Spectrum amp: 32
Integral amp: 80 (spec. amp. 2.5)
Solvent: CCl₄

ASSIGNMENTS

a ca 0.92 f 7.29
b 1.10-1.80 g _____
c 2.27 h _____
d 4.01 i _____
e 5.06



E 24M