(19) Europäisches Patentamt
European Patent Office
Office européen des brevets

(11) EP 0 856 573 A2

(12) EUROPEAN PATENT APPLICATION

(43) Date of publication:
05.08.1998 Bulletin 1998/32

(21) Application number: **98101355.0**

(22) Date of filing: **27.01.1998**

(51) Int. Cl.^{6}: **C10L 1/08**

(84) Designated Contracting States:
AT BE CH DE DK ES FI FR GB GR IE IT LI LU MC NL PT SE
Designated Extension States:
AL LT LV MK RO SI

(30) Priority: **29.01.1997 JP 29569/97**

(71) Applicant:
KABUSHIKI KAISHA TOYOTA CHUO KENKYUSHO
Aichi-gun Aichi-ken, 480-11 (JP)

(72) Inventors:
- **Nakakita, Kiyomi**
  Nishikamo-gun, Aichi-ken (JP)
- **Akihama, Kazuhiro**
  Kitaharayama-cho, Owariasahi-shi, Aichi (JP)
- **Mandokoro, Yoshiyuki**
  Nisshin-shi, Aichi-ken (JP)
- **Ogawa, Tadao**
  Kasugai-shi, Aichi-ken (JP)

(74) Representative:
Blumbach, Kramer & Partner GbR
Radeckestrasse 43
81245 München (DE)

(54) Diesel fuel composition for reduced particulate emission

(57) A diesel fuel composition for reduced particulate emission has a ^{13}C nuclear magnetic resonance (NMR) spectrum in which the ratio of the total area of a group of peaks with a chemical shift in the range of 33 to 50 ppm with respect to the total area of the group of peaks with a chemical shift in the range of 0 to 50 ppm is equal to or less than 30%, and preferably equal to or less than 20%. The region of the peaks with a chemical shift in the range of 33 to 50 ppm includes peaks due to at least a tertiary or quaternary carbon atom within saturated hydrocarbon portions with a branching structure. This diesel fuel composition has a reduced content of hydrocarbons with a branching structure and aromatic hydrocarbons, and is able to positively reduce the emission of particulate matter.

Printed by Xerox (UK) Business Services
2.16.3/3.4

Description

BACKGROUND OF THE INVENTION

FIELD OF THE INVENTION

The present invention relates to a diesel fuel composition which can yield reduced emissions of particulates (particulate matter) from a diesel engine.

RELATED ART

Particulates are one of the substances emitted from diesel engines which are subject to emission restrictions. Particulates consist principally of carbon particles (soot) and hydrocarbons and partially oxidized products resulting from incomplete combustion. A certain reduction in particulate emissions can be achieved by optimization of the combustion system of the diesel engine, but improvements in the diesel fuel are also required.

To reduce the particulate emissions by adapting the diesel fuel composition, it is known to be effective to reduce the content of distillate with a high boiling point, sulfur content, or density to increase cetane number, and to reduce the content of aromatic hydrocarbons, and in particular of polycyclic aromatic hydrocarbons. According to the researches of the inventors of the present application, however, it has become clear that the above countermeasures are not sufficient for particulate reduction.

SUMMARY OF THE INVENTION

An object of the present invention is to provide a diesel fuel composition with a reduced content of aromatic compounds which can realize further reduction of particulate emissions.

According to the researches of the present inventors, it has become clear that even a diesel fuel composition which has a reduced content of aromatic compounds and a lowered boiling point, does not necessarily yield a satisfactory reduction in particulate emissions. Furthermore, the present inventors have discovered that in addition to these two factors, the presence or absence of branch structures and the number of branches in hydrocarbons have a large effect on the generation of particulate matter, and have thus completed the invention.

In the diesel fuel composition for reduced particulate emission of the present invention, the ratio of the total area of a group of peaks with a chemical shift in the range of 33 ppm to 50 ppm with respect to the total area of a group of peaks with a chemical shift in the range of 0 ppm to 50 ppm is equal to or less than 30 % in a ^{13}C nuclear magnetic resonance spectrum (hereinafter referred to as "^{13}C-NMR spectrum").

In the ^{13}C-NMR spectrum, as described in more detail below, peaks with chemical shifts in the range of 0 to 50 ppm are due principally to carbon atoms constituting hydrocarbon portions not including unsaturated bonds, and peaks with chemical shifts in the range of 33 to 50 ppm are due principally to tertiary and quaternary carbon atoms within saturated hydrocarbon portions having branches, or carbon atoms adjacent to such atoms. And thus the total area of a group of peaks with a chemical shift in the range of 33 to 50 ppm corresponds to the presence or absence of branches, and the number of branches.

When the ratio of the total area of a group of peaks with a chemical shift in the range of 33 to 50 ppm with respect to the total area of the soup of peaks with a chemical shift in the range of 0 to 50 ppm is equal to or less than a specified value, which is specifically equal to or less than 30%, and more preferably equal to or less than 20%, the hydrocarbons in the diesel fuel composition having a branching structure can be reduced. As a result, the amount of particulate matter in the exhaust gas can be positively reduced.

In the diesel fuel composition of the present invention, the content of aromatic compounds is preferably equal to or less than 25% by volume, and even more preferably equal to or less than 20% by volume. By means of such a reduction in the content of aromatic compounds, the amount of particulate matter can be further positively reduced. Here, "aromatic compounds" include aromatic hydrocarbons and additives which include aromatic rings and so forth. And the aromatic compounds comprise polycyclic aromatic compounds and the content thereof is preferably equal to or less than 5 % by volume.

BRIEF DESCRIPTION OF THE DRAWINGS

Figs. 1A and 1B show ^{13}C-NMR spectra for a first embodiment and a first comparative example.

Figs. 2A to 2E illustrate molecular structures and chemical shifts corresponding to the peaks in the spectra shown in Figs. 1A and 1B.

Fig. 3 illustrates particulate measurements for the first embodiment and first comparative example.

Fig. 4 illustrates other particulate measurements for the first embodiment and first comparative example.

Fig. 5 shows the products of thermal decomposition and their concentrations obtained using a flow reactor, for the first embodiment and first comparative example.

Fig. 6 shows the products of thermal decomposition and their concentrations obtained using a flow reactor, for different isomers of hexane.

Fig. 7 is a graph showing the relationship between the initial reaction temperature and soot conversion ratio in Experiment 1 carried out with a shock tube.

Fig. 8 is a graph showing the relationship between the initial reaction temperature and soot conversion ratio in Experiment 2 carried out with a shock tube.

Fig. 9 is a graph showing the relationship between the initial reaction temperature and soot conversion ratio in Experiment 3 carried out with a shock tube.

Fig. 10 is a graph showing the relationship between the initial reaction temperature and soot conversion ratio in Experiment 4 carried out with a shock tube.

Fig. 11 is a graph showing the relationship between the initial reaction temperature and soot conversion ratio in Experiment 5 carried out with a shock tube.

Fig. 12 is a graph comparing the soot conversion ratios at the peaks respectively shown in Figs. 7 to 11.

DESCRIPTION OF PREFERRED EMBODIMENTS

The present invention is now described in terms of a preferred embodiment, with reference to specific data.

Figs. 1A and 1B show ^{13}C-NMR spectra, Fig. 1A being the spectrum for a diesel fuel composition embodying the present invention (first embodiment), and Fig. 1B the spectrum for a comparative diesel fuel composition (first comparative example).

In the ^{13}C-NMR spectrum of the present invention, the percentage ratio

$$\{(S2/S1) \times 100\}$$

of the total area **S2** of the group of peaks **e** with a chemical shift in the range of 33 to 50 ppm with respect to the total area **S1** of the group of peaks **P1** with a chemical shift in the range of 0 to 50 ppm is equal to or less than 30%, and preferably equal to or less than 20%. It should be noted that in Figs. 1A and 1B the group of peaks **P2** in the spectrum corresponds to the peaks for the solvent.

In the spectra of Figs. 1A and 1B, of the peaks belonging to group **P1**, the prominent peaks **a** to **d** correspond, as shown in Fig. 2A, to particular carbon atoms in unbranching saturated hydrocarbon portions. It should be noted that in Figs. 2A to 2E the numerals associated with particular carbon atoms indicate the corresponding chemical shifts. The peaks belonging to the group **e** with chemical shifts in the range of 33 to 50 ppm, as shown in part in Figs. 2B to 2E, correspond to tertiary and quaternary carbon atoms within branching molecules, or carbon atoms adjacent to such atoms. Molecular structures belonging to the group of peaks **e** are not limited to those shown in Figs. 2B to 2E, and many other examples exist. Moreover, this is well known, and is disclosed in the literature (for example, ^{13}C-NMR Data Book, edited by Fumio Toda and Tokio Oshima).

Specifically, in the hydrocarbons constituting diesel fuel, saturated hydrocarbon portions having tertiary or quaternary carbon atoms, for example hydrocarbons including alkyl groups (C_nH_{2n+1}), alkenyl groups (C_nH_{2n-1}), alkynyl groups and alkadienyl groups (C_nH_{2n-3}), and alkatrienyl groups (C_nH_{2n-5}), or the like, produce peaks with a chemical shift in the range of 33 to 50 ppm as above.

Table 1 shows the ratio of the area of each of the peaks **a** to **d** to the total peak area **S1**, and the ratio of the total peak area **S2** of the group of peaks **e** to the total peak area **S1** for the spectra of Figs. 1A and 1B. As is shown in Table 1, the proportion of the total peak area for the group of peaks **e** in the first embodiment of the present invention is 17.7%, whereas the proportion of the total peak area for the group of peaks **e** in the first comparative example is 30.5%.

Table 1

Sample	Peak Area Proportion (%)					
	Chemical Shift (ppm)	a 14	b 22	c 29	d 32	e 33-50
First Embodiment		9.0	11.2	31.6	8.3	17.7
First Comparative Example		6.7	9.7	17.0	6.0	30.5

Sample diesel fuel compositions used in experiments, and the results of analysis are now described.

Properties of the samples

Table 2 shows the properties of the diesel fuel composition of the first embodiment of the present invention and the first comparative example. The first comparative example is a commercial product (Sweden Class 1 diesel fuel (Shell Oil)), which with the object of reducing particulate emission has a low content of aromatic compounds and a reduced boiling point, compared with generally available commercial products.

The diesel fuel composition of the first embodiment with the object of reducing particulate emission also has a low content of aromatic compounds and a reduced boiling point, compared with generally available commercial products, but the content of aromatic compounds is about 10% higher by volume, and in the T50 to T90 range, the diesel fuel composition has boiling points of approximately 23 to 33 °C higher than those of the first comparative example. It should be noted that as a result of investigation of the combustion characteristics of these diesel fuel compositions, no large differences were found in the fuel-air mixture formation and flame development processes, ignition delay and heat release rate in both low and medium load ranges, and there are basically no differences in macroscopic combustion characteristics.

Table 2

		First Embodiment	First Comparative Example
Density (g/cm^3 at 15°C)		0.821	0.815
Cetane Index (JIS K 2204)		59	54
Cetane Number (JIS K 2280)		53	52
Viscosity (at 30°C)		2.989	2.390
Aromatic Content vol.% (IP 390/391)	Total	13.9	3.9
	Mono-	9.8	3.6
	Di-	3.4	0.3
	Tri-	0.7	ND
Sulfur Content wt%		0.06	0.00
Distillation Characteristics (°C)	Initial	186	184.5
	T5	209	-
	T10	221	202.5
	T20	232	212.5
	T30	242	221.5
	T40	251	229
	T50	259	236
	T60	268	243.5
	T70	277	250.5

	T80	287	259
	T90	304	271
	T95	316	281
	T97	322	-
	End	331	292
Hydrogen wt%		13.95	14.21
H/C		1.93	1.97
Calorific Value (kcal/kg)		10291	10312
Stoichiometric Air/Fuel Ratio		14.66	14.72

Particulate comparison

Next, measurements of the amount of particulate matter (PM) emitted under light load are shown in Figs. 3 and 4 for the first embodiment and first comparative example. Particulate matter comprises a soluble organic fraction (SOF), which is a component soluble in an organic solvent, and insoluble organic fraction (IOF), which is a component insoluble in an organic solvent and principally comprises soot. The particulate measurements may be made using the methods described in the literature, for example in F. Black, SAE Technical Paper 790422. It should be noted that Fig. 3 shows the case where the fuel injection timing is at a crank angle of degrees before top dead center, and Fig. 4 shows the case where the fuel injection timing is at a crank angle of 0 degrees, that is to say, at the top dead center. In both of Figs. 3 and 4, the bar indication **A** shows the results for the first embodiment and the bar indication **B** shows the results for the first comparative example.

From Figs. 3 and 4 it will be seen that the diesel fuel composition of the first embodiment exhibits a greatly reduced amount of particulate material, and particularly of insoluble organic fraction, compared with the diesel fuel composition of the first comparative example. That is to say, although the first comparative example has a highly reduced content of aromatic organic compounds and a highly lowered boiling point, the reduction in particulate emissions is not as effective as that of the first embodiment.

To investigate the reason for this contradictory result, analysis of the products of thermal decomposition of the diesel fuel compositions was carried out.

Analysis of the products of thermal decomposition

The products of thermal decomposition of two diesel fuels listed in Table 2 and obtained through a flow reactor were analyzed by a gas chromatography. The operating conditions of measurement in the flow reactor were as follows: nitrogen gas was used as the carrier gas, the sample was diluted 50 times by weight, the reaction time (time the gas was retained in the reaction tube) was 0.65 seconds, and the reaction temperature was 850°C.

Fig. 5 shows the concentrations of the products (acetylene, propadiene, benzene, and toluene) obtained by thermal decomposition of the diesel fuel compositions, using the flow reactor. Acetylene, propadiene, and other hydrocarbons with unsaturated bonds, and benzene, toluene, and other aromatic hydrocarbons are the substances which are the origin of the polycyclic aromatic hydrocarbons which are the precursors to particulate matter.

From Fig. 5 it is clear that the products of thermal decomposition of the diesel fuel composition of the first comparative example are produced in two to three times the quantity of those of the first embodiment. Thus, although the aromatic hydrocarbon content of the diesel fuel composition of the first comparative example has been greatly reduced, the substances which are the origin of the polycyclic aromatic hydrocarbons are produced in large quantities by thermal decomposition, and as a result the effect of reducing particulate emissions is lost, and if anything there can be an increase.

In this respect, a more detailed investigation was made of the influence of the presence or absence or the number of branches in hydrocarbons within a diesel fuel composition on the substances which are the origin of the polycyclic aromatic hydrocarbons which are the precursors to particulate matter, taking paraffins as an example.

Analysis of the influence of paraffin molecular structure on particulate generation

(1) Analysis of the effect of paraffin branching structure on the products of thermal decomposition using a flow reactor

Purpose:

In this experiment, in order to investigate the influence of paraffin branching structure within a diesel fuel composition on the generation of polycyclic aromatic hydrocarbon precursors which are the origin of particulate matter, from the viewpoint of the chemical properties of the diesel fuel composition, products of thermal decomposition by a flow reactor were analyzed. A number of simple paraffins with or without branches and of different numbers of branches were used as examples. Method of measurement:

Using a flow reactor in the same way as for the thermal decomposition of diesel fuel compositions described above, measurements were made under the same conditions except for the reaction temperature. More specifically the measurement conditions were as follows.

Carrier gas: nitrogen gas
Sample dilution: 50 times by weight
Reaction time: 0.65 seconds
Reaction temperature: 1000°C

As samples were used hexanes, with six carbon atoms. More specifically, three isomers were used: n-hexane, 2-methylpentane (i-hexane with one branch), and 2,2-dimethylbutane (i-hexane with two branches). Results:

The concentrations of products of thermal decomposition (acetylene, propadiene, benzene, and toluene) are shown in Fig. 6. From Fig. 6, it will be seen that for each of propadiene, benzene, and toluene, as the number of branches increases, these substances which are precursors to polycyclic aromatic hydrocarbons are produced in larger quantities. For acetylene, on the other hand, it will be seen that the number of branches has little effect.

(2) Analysis of the influence of the paraffin branching structure on the generation of soot, using a shock tube

Purpose:

In this experiment, in order to investigate the influence of paraffin branching structure within a diesel fuel on the generation of soot, from the viewpoint of the chemical properties of the diesel fuel composition, the amount of soot generated was measured in an ideal combustion field (field of spatially uniform and high temperature and pressure formed instantaneously) in a shock tube. A number of simple paraffins of different molecular structure were used as fuel. That is to say, the purpose of this experiment is to simplify the complicated phenomena occurring in a diesel engine, and prove chemically that the paraffin molecular structure has an effect on the amount of soot generated.

Experimental method:

A shock tube is a widely used device in the field of physical chemistry, as described in the literature (for example, Technopia, World Science Dictionary, published by Kodansha, Vol. 8, pp. 188-189, and M. Frenklach and S. Taki. A Conceptual Model for Soot Formation in Pyrolysis of Aromatic Hydrocarbons. Combustion and Flame 49. pp. 275-282, 1983). The shock tube used in this experiment was a stainless steel cylinder (outer diameter 89.1 mm, inner diameter 78.1 mm), and the lengths of the low pressure chamber (driven section) and the high pressure chamber (driver section) were 6 m and 3 m respectively.

In the experiment, first the low pressure chamber and the high pressure chamber were separated with an aluminum diaphragm, and the low pressure chamber and the high pressure chamber were evacuated to a vacuum, after which into the low pressure chamber was introduced as shown in Table 3 a test fuel gas diluted with argon, and the high pressure chamber was charged with helium as a driver gas, respectively at given pressures. Next the diaphragm was ruptured with an impact needle or spontaneously under the pressure of the high pressure chamber, whereby a shock wave was generated. A shock wave (the incident shock wave) advancing from the diaphragm toward the end wall of the low pressure chamber at the speed of sound or faster reached the end wall of the low pressure chamber and was reflexed, becoming a reflected shock wave. Behind this reflected shock wave, a high temperature field was instantaneously formed (duration approximately 1.5 ms), and thereby a reaction of the test fuel gas was caused, and soot was generated. It should be noted that the initial temperature of the reaction field generated by the reflected shock wave can be easily calculated from a measurement of the velocity of the incident shock wave into the low pressure chamber.

The amount of soot generated by the reaction was measured from the transmissivity of a helium neon laser passing through a pair of optical windows disposed at a distance of 1 cm from the end wall of the low pressure chamber. That is to say, using the fact that the transmissivity is reduced since the helium neon laser is attenuated by scattering by soot particles, the amount of soot can be determined. In this experiment, the benchmark used to indicate the amount of soot generated is the "soot conversion ratio" (proportion of the number of carbon atoms which are converted to soot particles to the total number of carbon atoms in the fuel of initial stage) defined by the well-known expression (1) from the measurement of the transmissivity of a helium neon laser. (For example, A. Alexiou and A. Williams. Soot Formation in Shock-Tube Pyrolysis of Toluene, Toluene-Methanol, Toluene-Ethanol, and Toluene-Oxygen Mixtures. Combustion and Flame 104. pp. 51-65, 1996)

$$\text{Soot conversion ratio} = (\text{total number of carbon atoms in soot}) / (\text{total number of carbon atoms in fuel initially behind reflected shock wave}) \quad (1)$$

The soot conversion ratio **t** seconds after the start of the reaction can be found, using the transmissivity **T(t)** of the helium neon laser measured in the experiment using the well-known expression (2).

$$\text{Soot conversion ratio} = (-N\rho\lambda \ln[T(t)])/(72\pi l E(m)[C]o) \quad \ldots \quad (2)$$

where

N: Avogadro's number
ρ: soot particle density
λ: wavelength of transmitted light
l: optical path length (78.1 mm: internal diameter of shock tube)
T(t): transmissivity at time **t**
[C]**o**: initial carbon concentration behind reflected shock wave

$$E(m) = -\mathrm{Im}[(m^2 - 1)/(m^2 + 2)]$$

m: complex refractive index of soot particles It should be noted that in this experiment a value of
E(m) = 0.253 was used.

In this experiment, as paraffins of different molecular structures were used five hexanes. Table 3 shows the composition of the (test fuel) gas charged in the low pressure chamber, the initial reaction temperature, the initial reaction pressure, and the initial carbon concentration behind the reflected shock wave.

It should be noted that the temperature behind the reflected shock wave (initial reaction temperature) was varied by adjusting the pressure of the propulsion gas (helium) charged in the high pressure chamber. In Table 3, in the composition of the gas charged in the low pressure chamber, the proportions of paraffin and oxygen are in a chemical equivalence ratio of 10, and this equivalence ratio is the condition corresponding to the excessively rich mixture portion in a diesel engine.

Table 3

I. Ex. No.	II. Composition of the Gas		III. Temperature (K)	IV. Pressure (atm)	V. [C]o (atoms/cc)
1	n-hexane Oxygen Argon	2.0 1.9 96.1	2100-2400	1.0-1.4	2.8×10^{17}
2	2-methylpentane Oxygen Argon	2.0 1.9 96.1	2150-2450		
3	3-methylpentane Oxygen Argon	2.0 1.9 96.1	2000-2500		
4	2,2-dimethylbutane Oxygen Argon	2.0 1.9 96.1	2100-2450		
5	2,3-dimethylbutane Oxygen Argon	2.0 1.9 96.1	2150-2500		

I: Experiment Number

II: Composition of the (Test Fuel) Gas Charged in the Low Pressure Chamber (vol. %)

III: Initial Reaction Temperature (K)

IV: Initial Reaction Pressure (atm)

V: Initial Carbon Number Density Behind the Reflected Shock Wave [C]o (atoms/cc)

Results:

The results are shown in Figs. 7 to 11. In Figs. 7 to 11, the horizontal axis represents the temperature (initial reaction temperature) behind the reflected shock wave, and the vertical axis represents the soot conversion ratio 1 millisecond after the start of the reaction. All the results exhibit characteristics which reach a maximum soot conversion ratio at a particular temperature, that is to say, bell curves.

Fig. 12 shows a comparison of the peak values of the bell curves shown in Figs. 7 to 11. Compared with the n-hexane (zero branches) in experiment number 1, the methylpentane (i-hexane with one branch) in experiments number 2 and 3, and the dimethylbutane (i-hexane with two branches) in experiments number 4 and 5 exhibit progressively higher values of the soot conversion ratio (soot production capacity). That is to say, the soot production capacity increases as the number of branches increases. From comparisons of experiments number 2 and 3 and experiments number 4 and 5, however, the position of the branches has only a small effect on the soot production capacity.

From the above it is seen that:

(1) Soot is more easily generated from branching paraffins than from unbranching paraffins; and
(2) The soot production capacity is little influenced by the position of the branches within the paraffin, and is largely determined by the number of branches.

Thus, the influence over the production of soot exerted by the molecular structure of paraffins in a diesel fuel composition has been chemically confirmed by the above experiments, where the effects of complicated phenomena inside the diesel engine have been eliminated.

Claims

1. A diesel fuel composition for reduced particulate emission, comprising hydrocarbons having a ^{13}C nuclear magnetic resonance spectrum wherein the ratio of the total area of a group of peaks with a chemical shift in the range of 33 ppm to 50 ppm with respect to the total area of a group of peaks with a chemical shift in the range of 0 ppm to 50 ppm is equal to or less than 30 %.

2. The diesel fuel composition for reduced particulate emission as defined in claim 1,
   wherein said ratio of the total area of a group of peaks with a chemical shift in the range of 33 ppm to 50 ppm with respect to the total area of a group of peaks with a chemical shift in the range of 0 ppm to 50 ppm is equal to or less than 20 %.

3. The diesel fuel composition for reduced particulate emission as defined in claim 1 or 2,
   wherein said hydrocarbons comprise 25 % by volume or less of aromatic compounds.

4. The diesel fuel composition for reduced particulate emission as defined in claim 1 or 2,
   wherein said hydrocarbons comprise 20 % by volume or less of aromatic compounds.

5. The diesel fuel composition for reduced particulate emission as defined in claim 3 or 4,
   wherein said aromatic compounds comprise polycyclic aromatic compounds and the content thereof is equal to or less than 5 % by volume.

FIG. 1A

FIG. 1B

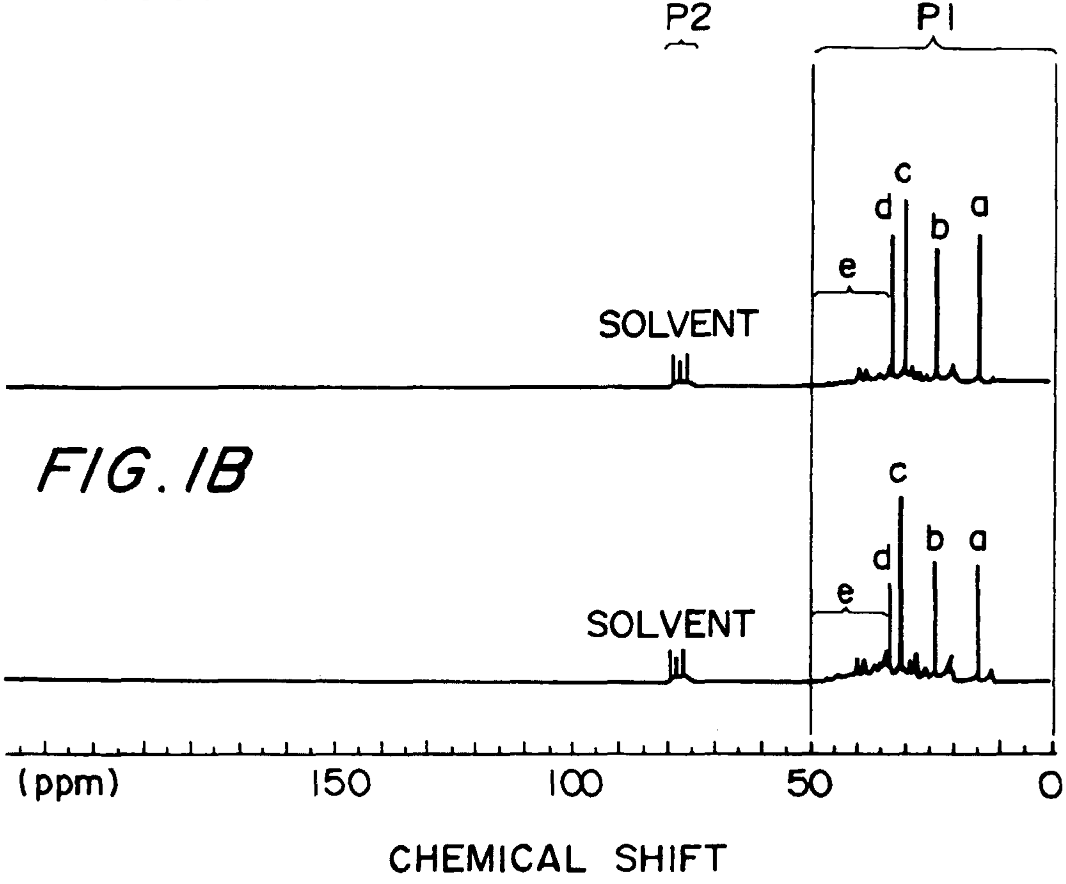
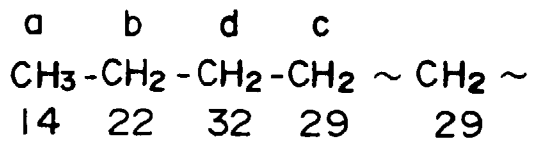
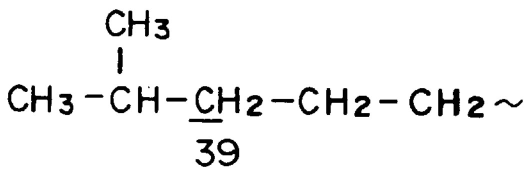

P2
P1
c
d
b
a
e
SOLVENT
c
b
a
d
e
SOLVENT
(ppm)
150
100
50
0
CHEMICAL SHIFT

FIG. 2A



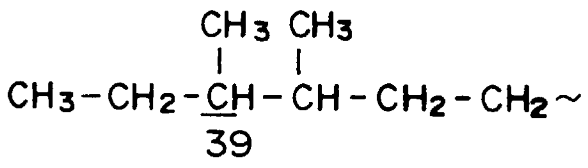
$$\underset{14}{\overset{a}{CH_3}}-\underset{22}{\overset{b}{CH_2}}-\underset{32}{\overset{d}{CH_2}}-\underset{29}{\overset{c}{CH_2}}\sim\underset{29}{CH_2}\sim$$

FIG. 2B



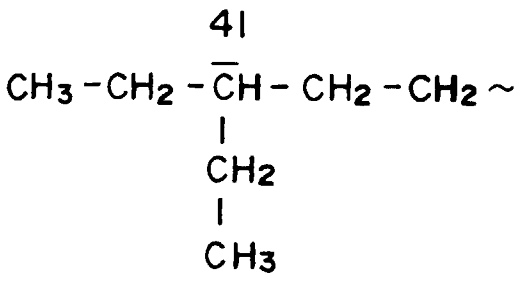
$$CH_3-\overset{\substack{CH_3\\|}}{CH}-\underset{39}{\underline{C}}H_2-CH_2-CH_2\sim$$

FIG. 2C



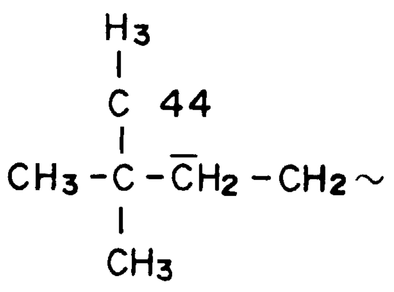
$$CH_3-CH_2-\overset{\substack{CH_3\\|}}{\underset{39}{\underline{C}}H}-\overset{\substack{CH_3\\|}}{CH}-CH_2-CH_2\sim$$

FIG. 2D



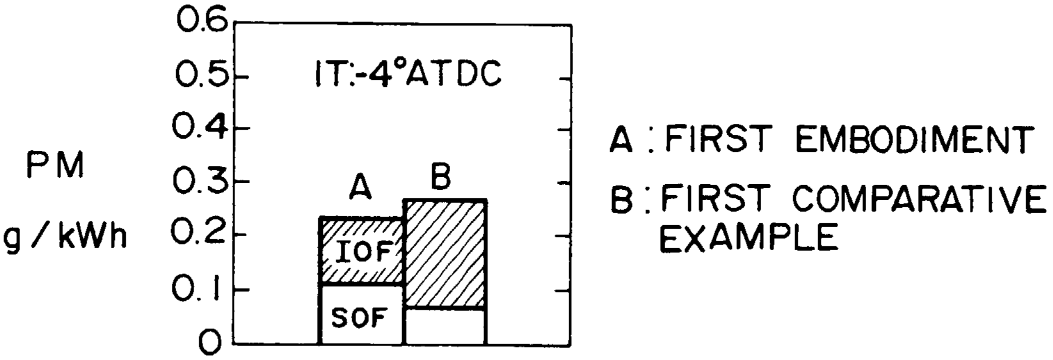
$$CH_3-CH_2-\underset{\substack{|\\CH_2\\|\\CH_3}}{\overset{41}{\overline{C}H}}-CH_2-CH_2\sim$$

FIG. 2E



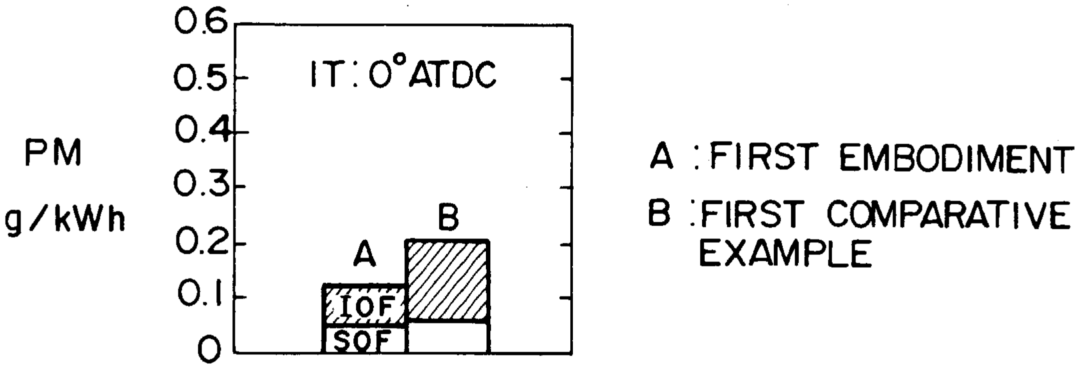
$$CH_3-\overset{\substack{H_3\\|\\C\quad 44\\|}}{\underset{\substack{|\\CH_3}}{C}}-\overline{C}H_2-CH_2\sim$$

FIG. 3



(1800rpm, ϕ:0.29, Pinj:40MPa)

FIG. 4



(1800rpm, ϕ:0.29,Pinj:40MPa)

FIG. 5

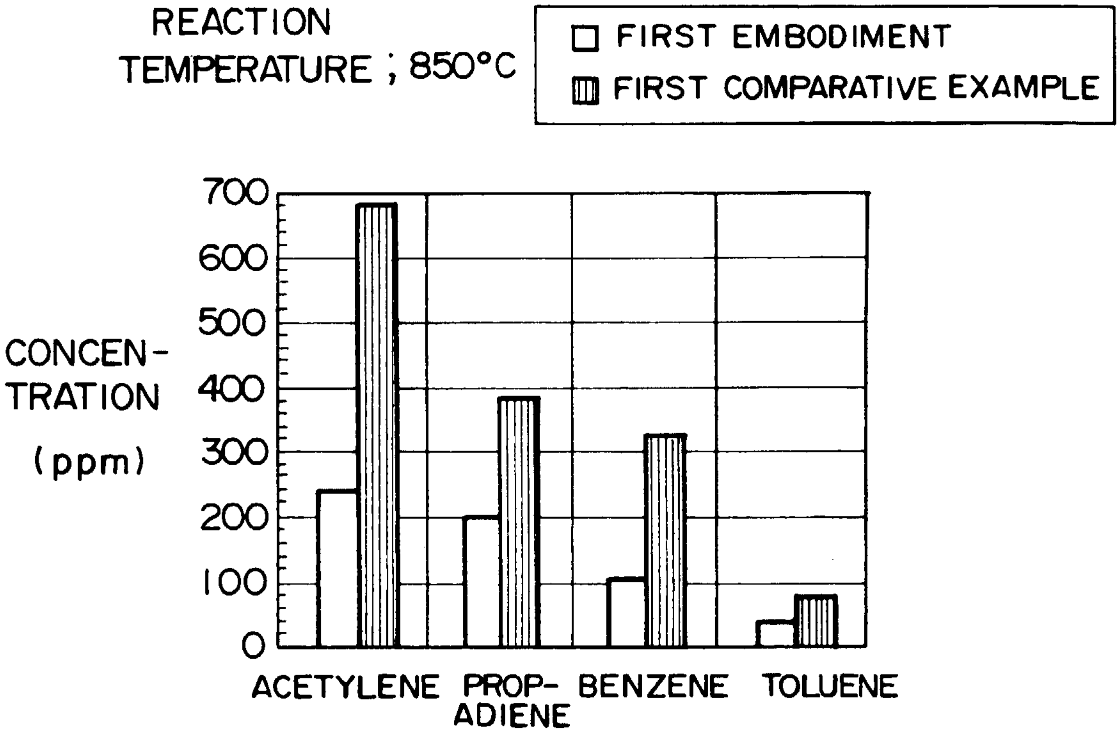

REACTION
TEMPERATURE ; 850°C
□ FIRST EMBODIMENT
▥ FIRST COMPARATIVE EXAMPLE
CONCEN-
TRATION
(ppm)
700
600
500
400
300
200
100
0
ACETYLENE
PROP-
ADIENE
BENZENE
TOLUENE

FIG. 6

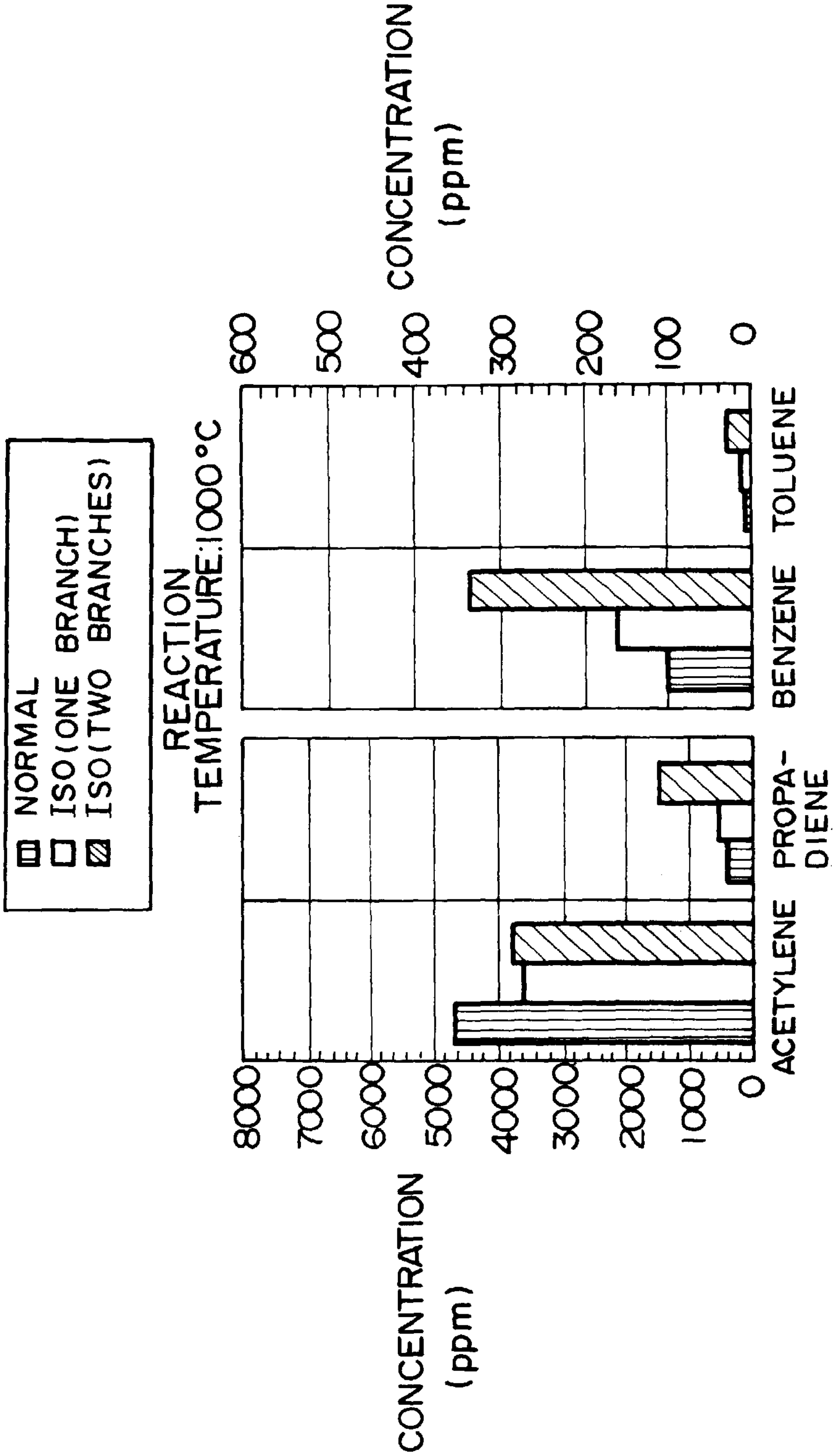

▤ NORMAL
☐ ISO(ONE BRANCH)
▨ ISO(TWO BRANCHES)
REACTION TEMPERATURE:1000°C
CONCENTRATION (ppm)
8000
7000
6000
5000
4000
3000
2000
1000
0
ACETYLENE
PROPA-DIENE
BENZENE
TOLUENE
CONCENTRATION (ppm)
600
500
400
300
200
100
0

FIG. 7

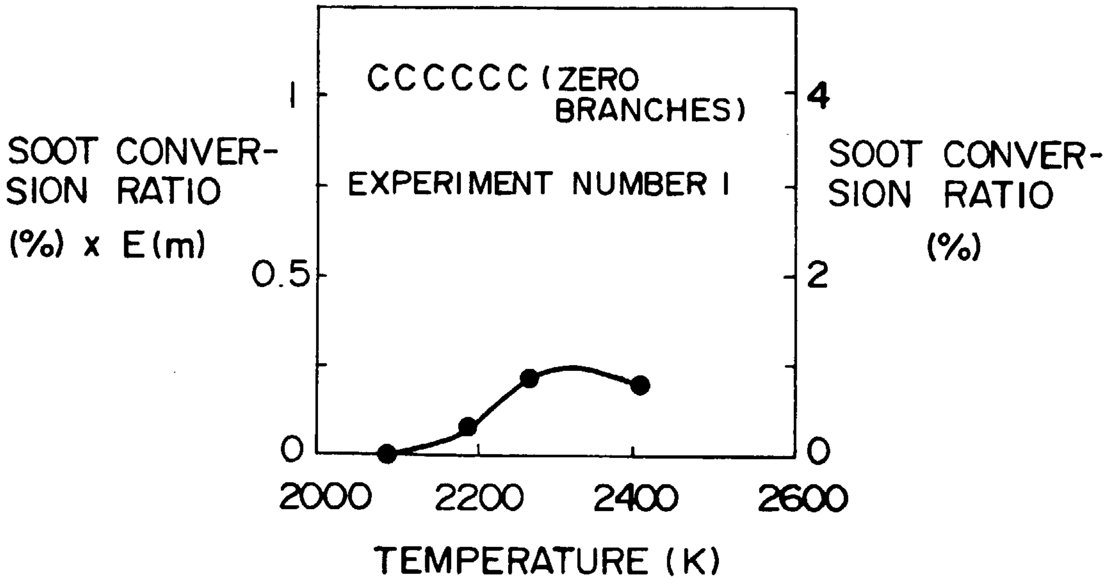

CCCCCC (ZERO BRANCHES)
EXPERIMENT NUMBER 1
SOOT CONVERSION RATIO (%) x E(m)
SOOT CONVERSION RATIO (%)
1
0.5
0
4
2
0
2000
2200
2400
2600
TEMPERATURE (K)

FIG. 8

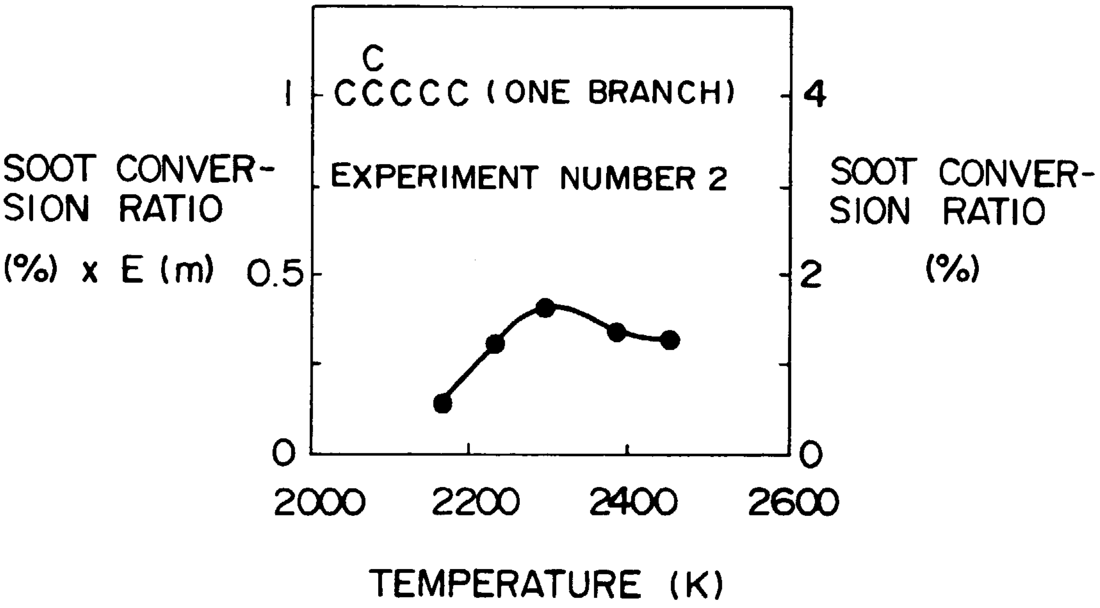
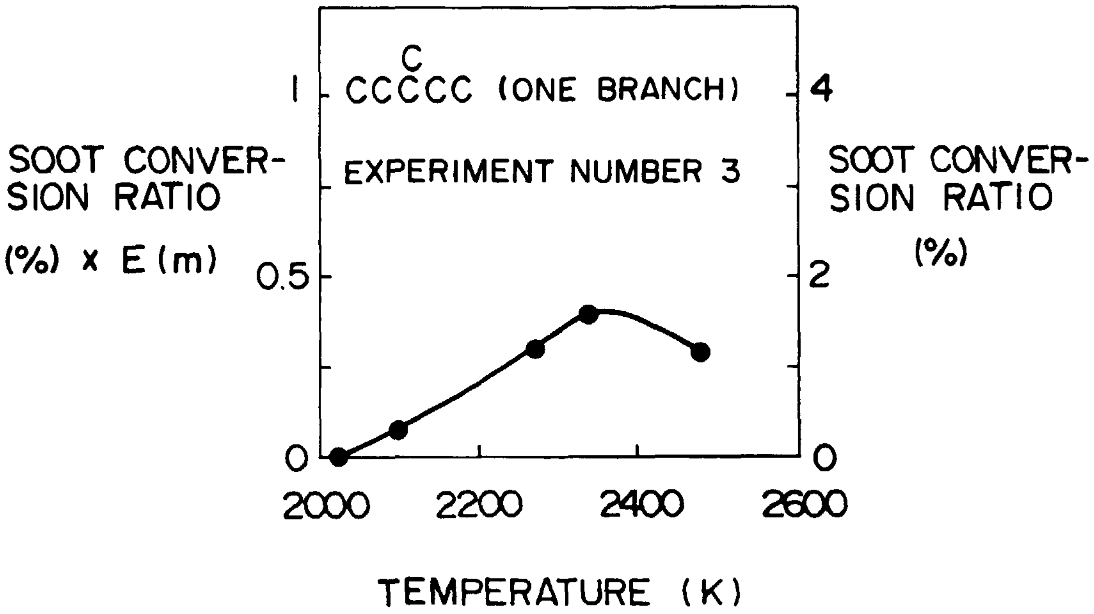
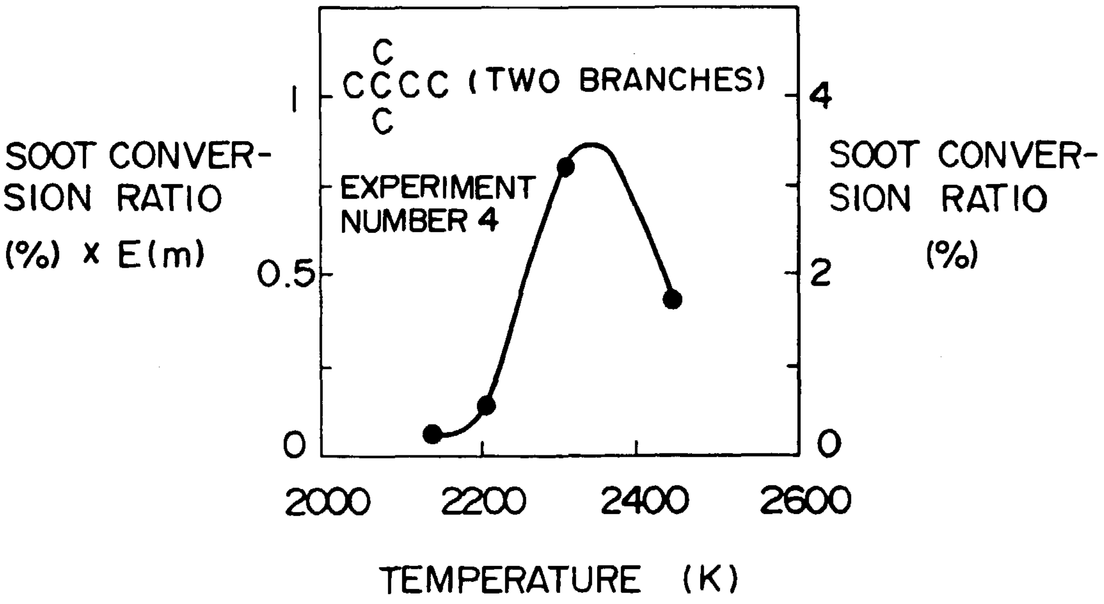

C
CCCCC (ONE BRANCH)
EXPERIMENT NUMBER 2
SOOT CONVERSION RATIO (%) x E (m)
SOOT CONVERSION RATIO (%)
1
0.5
0
4
2
0
2000
2200
2400
2600
TEMPERATURE (K)

FIG. 9



C
CCCCC (ONE BRANCH)
EXPERIMENT NUMBER 3
SOOT CONVERSION RATIO (%) x E(m)
1
0.5
0
SOOT CONVERSION RATIO (%)
4
2
0
2000
2200
2400
2600
TEMPERATURE (K)

FIG. 10



C
CCCC (TWO BRANCHES)
C
EXPERIMENT NUMBER 4
SOOT CONVERSION RATIO (%) x E(m)
1
0.5
0
SOOT CONVERSION RATIO (%)
4
2
0
2000
2200
2400
2600
TEMPERATURE (K)

FIG. 11

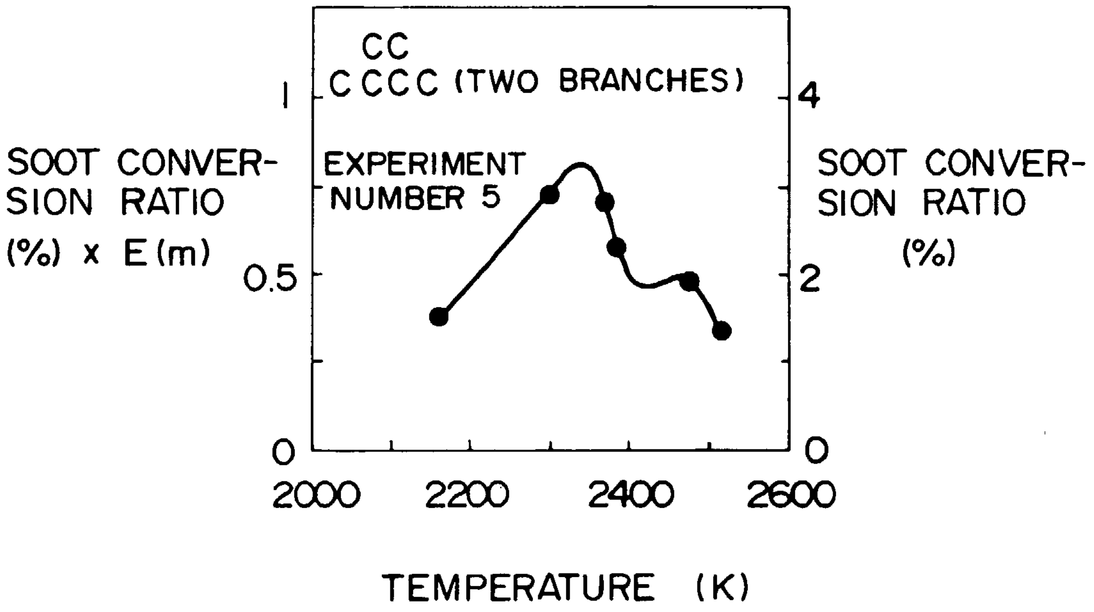
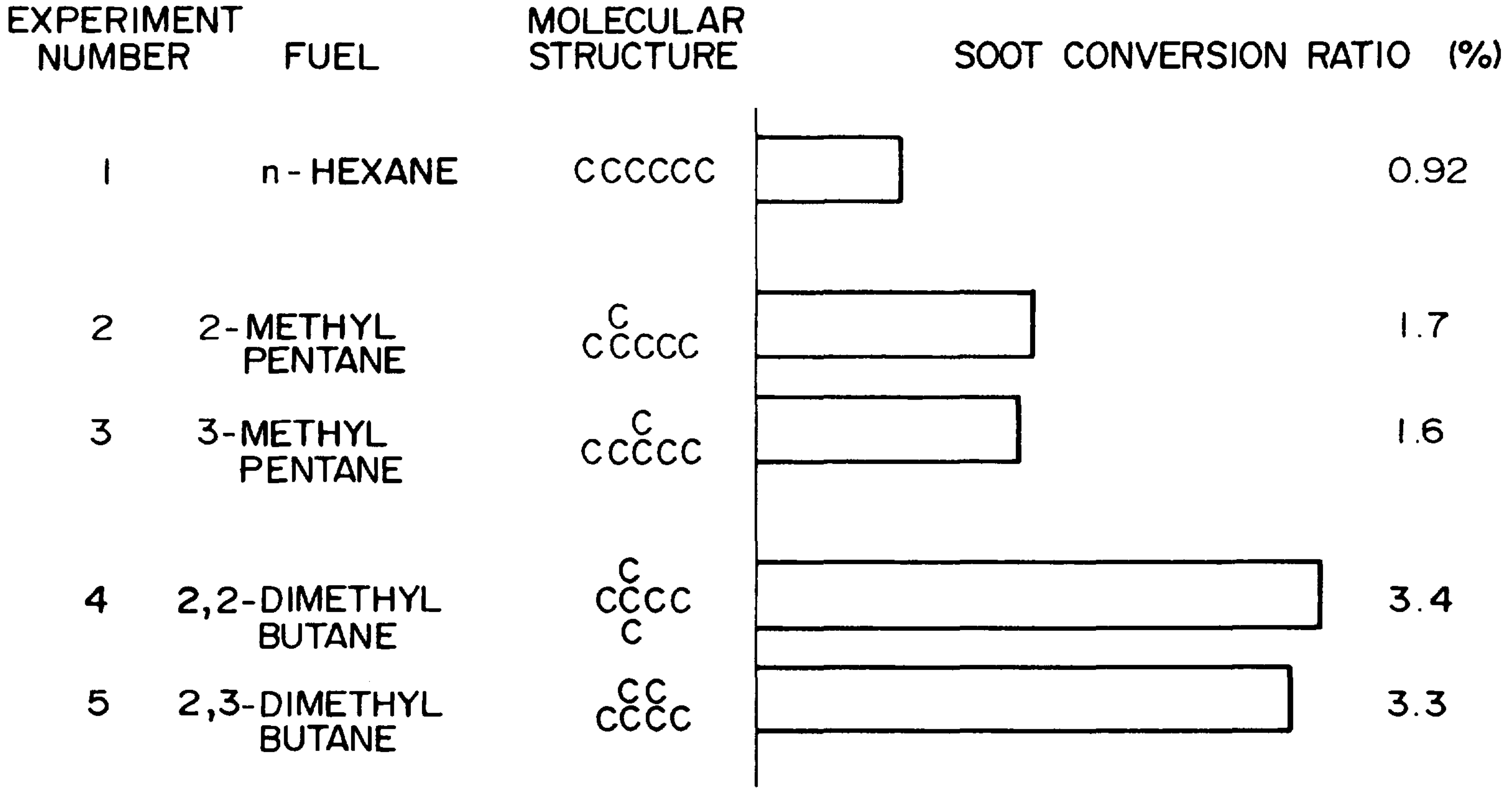

CC
CCCC (TWO BRANCHES)
EXPERIMENT NUMBER 5
SOOT CONVERSION RATIO (%) x E(m)
SOOT CONVERSION RATIO (%)
1
0.5
0
4
2
0
2000
2200
2400
2600
TEMPERATURE (K)

FIG. 12



EXPERIMENT NUMBER	FUEL	MOLECULAR STRUCTURE	SOOT CONVERSION RATIO (%)
1	n-HEXANE	CCCCCC	0.92
2	2-METHYL PENTANE	C CCCCC	1.7
3	3-METHYL PENTANE	C CCCCC	1.6
4	2,2-DIMETHYL BUTANE	C CCCC C	3.4
5	2,3-DIMETHYL BUTANE	CC CCCC	3.3