

## COAL STRUCTURE VS. FLASH PYROLYSIS PRODUCTS

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The fast pyrolysis of coal produces tar, char and a range of low molecular weight gases in various proportions and amounts depending on the pyrolysis conditions (temperature, pressure) and the coal being pyrolyzed. Much research effort has been devoted to study of the reaction kinetics and effect of process variables, attempting thereby to elucidate the pyrolysis mechanism<sup>(1)</sup>. Less effort has been focused on coal chemical structure and its relationship to the pyrolysis reactions and pyrolysis products. It was to attempt to better understand coal structure and its influence on pyrolysis products and pyrolysis mechanisms that this project was undertaken. This paper will report only on that portion of the work concerned with the aliphatic hydrocarbon products and particularly the light olefins.

A continuous bench-scale pyrolysis apparatus (Fig. 1) was constructed similar to the design of Tyler<sup>(2)</sup>. The coal entrained in a nitrogen stream was injected into a sand bed fluidized with nitrogen and heated in a split furnace to the temperature desired. Volatiles emitted from the sand bed were passed into two cold traps in series containing cellulose thimbles to filter out the tar and char from the off-gas. Gas exiting the cold traps was vented through a wet-test meter with a side stream entering a Perkin-Elmer Sigma One computer-controlled gas chromatograph which analyzed for some 16 components. At the end of a pyrolysis run, the tar and char caught in the two thimbles were extracted in a soxhlet extractor with methylene chloride and methanol to obtain the weight of tar and char produced.

Figure 2 shows tar yields vs. temperature for a Texas Lignite. Figure 3 shows how the quantity and composition of the pyrolysis gas from the same coal varies with temperature. Only the major gases are shown. These curves are typical of many coals although the actual quantities vary<sup>(3)</sup>. From these two figures, it is apparent that the tar produced goes through a maximum at about 600°C and up to that temperature relatively small amounts of gases are evolved. Above 600°C, the production of the various gases increases rapidly while at the same time, the tar yield drops off. The inference can be drawn that the gas is coming from tar pyrolysis. That this is so, can be shown by pyrolyzing tar which has been produced at 600°C, at higher temperatures. Similar gaseous products are produced and in similar ratio as when coal is pyrolyzed at the higher temperature<sup>(4)</sup>.

The yields of the hydrocarbon gases produced on coal pyrolysis vary greatly depending on the particular coal. This is shown for ethylene, one of the major products, in the first two columns of Table 1. The ethylene yield is related to the propylene

yield as shown by Figure 4. Similarly, the ethylene yield is related to the butadiene yield, suggesting that these gases have a common precursor. The methane and benzene, however, show no obvious relation to the ethylene yields. These products are apparently derived mainly from other components in the coal.

#### Coal Structure vs. Pyrolysis Products

To try to relate these yield differences to structural differences in the coals themselves, each coal whose pyrolysis behavior was studied was examined by  $^{13}\text{C}$  NMR (with cross polarization and magic angle spinning). This work was done by E. A. Hagaman and H. Zeldes of Oak Ridge National Laboratory in a cooperative program with Du Pont. Typical pattern differences between a high ethylene-producing coal (PSOC 124), a low ethylene-producing bituminous coal (Sewickley) and two intermediate coals (Con Paso Blue 2 and PSOC 181), are shown in Figure 5. While the PSOC 124 coal shows high aliphatic character and the Sewickley shows the expected higher aromaticity, various other evidence suggests that aliphatic character alone is not the determining factor. The fractional area representing a chemical shift at 31 ppm, however, which is associated with methylene chains greater than 5 or 6 segments long, appears to correlate with the ethylene yield results. This peak which occurs at a chemical shift of 29 ppm in substances in solution is apparently shifted slightly to 30-32 ppm in solid coal. This was shown by running stearic acid in solution, and impregnated on to anthracite coal. The 29 ppm peak was shifted up field and broadened on the coal.

A plot of ethylene yield vs. the area fraction of the  $^{13}\text{C}$  NMR spectrum at a chemical shift of 31 ppm, times the weight fraction of carbon in the coal is shown in Figure 6. The line is the least-squares fit to the points shown. While there is scatter in the data, a correlation is apparent (Correlation coefficient = .92).

#### Tar Structure Studies

Low temperature (600°C or less) pyrolysis of coal produces high yields of tar which on further pyrolysis produces the volatile hydrocarbon products we observe on high-temperature pyrolysis of coal. This shows that this tar contains the aliphatic precursors we observe in the coal itself, although they may be changed somewhat from the form in which they are in the coal. A number of tars were therefore produced by pyrolysis of several different coals at 600°C in the laboratory coal pyrolysis unit for further study.

A  $^{13}\text{C}$  NMR pattern for a solution of Millmerran tar (10% in  $\text{CDCl}_3$ ) from 600°C pyrolysis is shown in Figure 7. It shows a very strong peak at a chemical shift of 29 ppm. The  $^1\text{H}$  NMR spectrum was run on the same tar in  $\text{CDCl}_3$  solution (Figure 8). It shows a strong peak at 1.2 ppm known to be due to methylene chains over 5 units long. By using a Dow Corning silicone DC200 fluid ( $\% \text{H} = 8.06$ ) internal standard in the  $\text{CDCl}_3$  solvent, quantitative determination of the  $(\text{CH}_2)_n$  peak by ratio of its area to that of the 0 ppm silicone peak was possible. This showed 33.6 wt. %  $(\text{CH}_2)_n$  in the tar. Similar patterns are shown by tars of other coals.

To quantify the assignment of the 1.2 peak in the proton NMR spectrum, a series of model compounds having long methylene chains was dissolved in  $\text{CDCl}_3$  containing the silicone internal standard. In all cases, the 1.2-1.3 peak was very large and clearly detectable. Weight %  $(\text{CH}_2)_n$  calculated for each compound are shown in Table 2. As can be seen from the Table, not all methylene groups appear in the proton NMR spectrum at 1.2-1.3 ppm. Only those  $(\text{CH}_2)$  groups shown in brackets in the structural formulas show up at that place. Those  $\text{CH}_2$  groups conjugated with or close to the carboxyl groups or benzene rings appear at higher chemical shifts, and methyl groups appear at 0.7-0.8 ppm. This clearly identifies the 1.2-1.3 ppm peak as due to  $(\text{CH}_2)_n$  but at the same time indicates that any analysis based on this method will not include all of the  $(\text{CH}_2)$  groups in coal. If the chains are long, however, most of the methylene will be included.

Table 3 shows the distribution of types of protons in 600°C pyrolysis tars from four different coals representing a wide range of olefin yields on pyrolysis. The Table shows that roughly 35% of the protons in the tar are polymethylene protons, the rest are divided between methyl groups, hydroaromatic hydrogens, hydrogens attached to aromatic carbons, and a small number of olefinic and some unidentified protons.

Table 4 shows the distribution of protons in tar from Texas Lignite pyrolyzed at various temperatures from 600°C to 920°C. This clearly shows that as the pyrolysis temperature is increased, the content of polymethylene in the tar decreases as do the hydroaromatic hydrogens. The aromatic hydrogens on the other hand increase rapidly to become the predominant species. This provides a convenient measure of the completeness of pyrolysis.

To try to isolate and purify larger quantities of the hydrocarbon precursors, a separation was made of the Millmerran tar by Preparative Liquid Chromatography. A number of fractions across the chromatogram were analyzed by FTIR and  $^1\text{H}$  NMR and fraction 21 representing 38% of the original sample turned out to be high in  $(\text{CH}_2)_n$  (concentration 68%). An Infrared spectrum of that fraction (Figure 9) showed a well resolved peak at  $720\text{cm}^{-1}$ , known to be characteristic of long methylene chains. This peak has a low extinction coefficient and is rarely discernible above background in coals themselves. A GC/MS pattern of that fraction (Figure 10) shows olefin/paraffin pairs of peaks from  $\text{C}_{17}$  to  $\text{C}_{24}$ .

The polymethylene compounds in pyrolysis tars are mainly present as linear paraffins or olefins, however, there are indications of lesser amounts of branched paraffins and olefins and alkylaryl compounds as well in the unfractionated tars. The form the polymethylene compounds have in the coal itself is not known, but extraction of various coals with methylene chloride for several days failed to remove more than 1% of the material, suggesting that the major part of the polymethylene compounds may be either chemically combined in the coal structure or else trapped.

#### Model Compound Pyrolysis

While it seemed likely on the basis of petroleum experience that polymethylene compounds would pyrolyze to form the low molecular

weight aliphatic hydrocarbons we observe on coal pyrolysis, known compounds as models of polymethylene and other structures in coal were pyrolyzed at similar temperatures and contact times as the coal.

Table 5 summarizes the results of pyrolysis of 7 model compounds. Products are only shown as major and minor. As can be seen by referring to the Table, under the pyrolysis conditions used, compounds containing methylene chains such as dodecane, octadecane, stearic acid, ethylbenzene, propylbenzene, butylbenzene, and phenyl-dodecane on cracking give substantial quantities of ethylene along with butadiene, propylene and other hydrocarbons in amounts roughly comparable to what we observe in coal pyrolysis. The aromatic portion in alkylaryl compounds appears to go mainly to toluene although small amounts of benzene and some styrene are produced as well. Some methane is also produced along with minor amounts of ethane, butane and other hydrocarbon. These results are quite consistent with what we find in coal pyrolysis and with petroleum cracking technology.

Interestingly, the methylaryl compounds investigated thus far do not produce methane on pyrolysis under the conditions we used. Toluene and the three xylene isomers apparently are only slightly converted at 850°C and 0.5 to 1.0 second contact time in the sand bed. 9-Methylantracene and 3,6-dimethylphenanthrene produced no methane or other gaseous products, although they appeared to form tar or coke. This is consistent with the observations of Lang et al on methyl-naphthalenes(5) which form condensation products but not gases under pyrolysis conditions.

#### Analysis for Polymethylene in Coal Itself

With  $^{13}\text{C}$  NMR indication of the  $(\text{CH}_2)_n$  moiety in coal and evidence of  $(\text{CH}_2)_n$  in low and high temperature<sup>n</sup> pyrolysis tars, as well as model compound pyrolysis information, it seemed important to devise a quantitative analytical method for  $(\text{CH}_2)_n$  in coal itself. This raised the question whether coal could be liquefied under generally accepted solvent refining conditions and still retain undecomposed the polymethylene component? Also, if the  $(\text{CH}_2)_n$  is liberated but not destroyed, can it be detected and quantitatively determined by proton NMR?

Figure 11 shows the proton NMR pattern of the liquefaction product of PSOC 124, a high ethylene yielding coal which was liquefied using 3 grams of coal, 3 grams of tetralin as donor solvent, 0.1 gram each of sodium sulfide and ferrous sulfide as liquefaction catalysts and 2000 psi pressure (cold) of hydrogen in a 10 ml shaker bomb. The liquefaction was run at 425°C for 2 hours in a sand bath with vertical shaking. The product liquid was washed out of the shaker tube with methylene chloride and filtered to remove the solids (ash, unconverted coal and catalysts). After removal of the  $\text{CH}_2\text{Cl}_2$  by distillation, a weighed sample of the liquid was dissolved in deuterio-chloroform containing a known amount of DC200 silicone fluid as internal standard. Examination of the NMR pattern clearly shows the  $(\text{CH}_2)_n$  peak at 1.2 ppm and the  $\text{CH}_3$  peak at about 0.8 ppm indicating that the polymethylene component of the coal is released from the coal matrix but not destroyed in the liquefaction process.

The rest of the NMR pattern (beyond 1.3 ppm) is heavily affected by the presence of the donor solvent and its dehydrogenation products so that this method is only useful for detecting the  $(CH_2)_n$ .

To develop a routine analysis based on coal liquefaction, first a series of batch shaker tube liquefaction runs were made in 10 ml shaker tubes using the same recipe as previously but varying the time, temperature and donor solvent. Tests were made with three different donor solvents [tetralin, dihydrophenanthrene (DHP), and tetrahydroquinoline (THQ)]. The  $(CH_2)_n$  figures on the right hand 5 columns of Table 6 were obtained by separating the liquid from the solid by extraction with  $CH_2Cl_2$ , filtration to remove the solids, and distilling off the solvent ( $CH_2Cl_2$ ). The  $(CH_2)_n$  content of the liquid was determined by dissolving a weighed sample of liquid into a volumetric flask and making up to the line with  $CCl_3D$  containing a known quantity of DC-200 silicone internal standard. All conversions were 85% or more and usually above 90%.

In most cases, all three donor solvents gave similar results, but in a few cases the tetrahydroquinoline gave higher values. THQ was, therefore, selected for further investigation. Liquefactions were run, varying temperature and contact time. These results are shown in the three right-hand columns of Table 6 where results were reported for 400°C and 1.65 hours and 435°C for 4 hours. The lower temperature short contact time liquids were viscous and hard to work up. The high temperature longer time reactions showed little change over the 425°C/2 hour samples, so the latter conditions were selected as optimum.

The values obtained for  $(CH_2)_n$  content of coals from coal liquefaction are reasonable based on the amount of ethylene produced in pyrolysis shown in column 1 and ethylene plus other hydrocarbons believed to come from the same source shown in column 2 of Table 6. These should represent minimum amounts in the coal. Column 3 shows the  $(CH_2)_n$  found in pyrolysis tars calculated on the basis of the original coal which should also be a minimum since not all the tar is driven out of the coal at 0.5 seconds pyrolysis contact time.

For a number of reasons, it was desirable to be able to run this liquefaction analysis on a micro (<10 mg) scale. This would be much simpler to do if no added catalyst was required and hydrogen pressure was not needed. Experiments were, therefore, tried to see whether such an analysis could be developed under those conditions. Liquefactions were run in 3" long 3 mm pyrex glass tubes. Approx. 5 mg of (-200 mesh) coal samples (weighed to .01 mg) were charged to the tubes along with 10 mg of calcined clean sand, 1.1 times the weight of coal of the donor solvent and a 1 cm long 2 mm glass rod (for agitation) and the tubes purged with nitrogen and sealed.

Two such tubes were packed into each 10 ml shaker tube with steel wool packed around them. They were then subjected to 425°C for 2 hours in a sand bath with rapid vertical agitation with approximately 5 minutes heat up time to temperature and rapid cool down in a cold air stream.

The tubes were worked up by breaking in the middle and rinsing repeatedly with  $\text{CCl}_3\text{D}$  containing a weighed amount of DC-200 fluid, through a glass wool plug filter into a 1 ml volumetric flask. The contents of the flask were put into an NMR tube and run on the IBM NR-80 Fourier Transform NMR Spectrometer. The area of the 1.2 ppm peak was determined relative to the silicone peak and the weight %  $(\text{CH}_2)_n$  calculated using the area ratio.

The results of these experiments are shown in columns 1, 2 and 3 in Table 7. They clearly show that low results are obtained with tetralin and dihydrophenanthrene under these conditions. This may be due in part to lower donor activity, but more likely due to low hydrogen content of the donor in the absence of a hydrogen atmosphere. The results with tetrahydroquinoline, however, appear to be about the same whether in the micro mode without hydrogen pressure or catalyst or in the macro mode with both. This system was, therefore, adopted as being simple, rapid and giving results equivalent to the macro system. Analysis of pairs of samples from some 40 coals by this method ranging in %  $(\text{CH}_2)_n$  content by weight of from 0 to 17% (MF) showed a standard deviation of 0.59%. Table 1 column 3 shows these values for the coals previously discussed together with the ethylene yields. In view of the sampling problems with a heterogeneous material like coal and the small sample size, analyses were normally run in pairs. The coal was ground fine (-200 mesh) and well blended. Where greater accuracy is desired, more replicates can be easily run and the  $^1\text{H}$  NMR can be run with more scans.

Ethylene yields (850°C) vs.  $(\text{CH}_2)_n$  concentration for these coals are plotted in Figure 12 with the linear regression line shown. A correlation coefficient of 0.952 and a 0 intercept shows a good correlation.

Similarly plots of propylene and butadiene yields for the same coals, vs.  $(\text{CH}_2)_n$  content also show strong correlations.

### Conclusions

We conclude from the experiments described that the low molecular weight aliphatic hydrocarbons produced by flash pyrolysis of coal at temperatures of 700°C and over, result primarily from the cracking of long methylene chains which are part of the coal structure or trapped in it. Low temperature (600°C) pyrolysis of the coal drives off a portion of the coal as tar which contains these polymethylene moieties, primarily in the form of normal paraffins and olefins from  $\text{C}_{17}$  to  $\text{C}_{24}$  and higher. This polymethylene precursor(s) in coal is apparently destroyed during coalification, as it is essentially absent in anthracite and is much higher in lignite and subbituminous coals. However, even in low rank coals the concentration of the polymethylene moiety varies widely, probably determined by the types of plants from which the coals are derived. Cannel coals generally contain fairly large amounts of  $(\text{CH}_2)_n$  (up to 17% or more). Some lignites and subbituminous coals contain as much as 10%  $(\text{CH}_2)_n$ .

Several other investigators (6-15) have reported the presence of aliphatic hydrocarbons in coal based mainly on solvent extractions. The amounts reported, however, have been generally much less than was found in this work. The difference presumably is that most of the polymethylene is chemically bound or trapped and non-extractable. Deno<sup>(16)</sup> reported the presence of long chain methylene compounds by chemical degradation of the coal, however, no quantitative conclusions could be drawn from that work.

The liquefaction method for estimation of  $(CH_2)_n$  content of coals is being used to determine the  $(CH_2)_n$  content of coal macerals and to explore the geochemical origins of the polymethylene components in coal.

#### Acknowledgements

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FIGURE 1  
 -1 GM/HR COAL PYROLYSIS UNIT

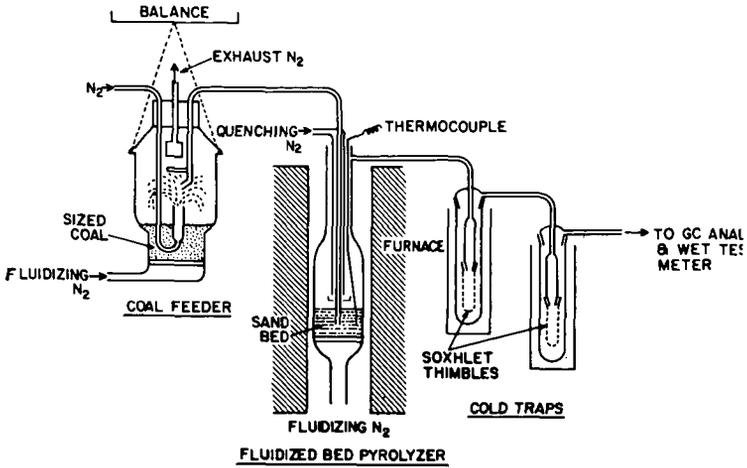


FIGURE 2

PRODUCT YIELDS FROM THE FLASH PYROLYSIS  
 OF TEXAS LIGNITE

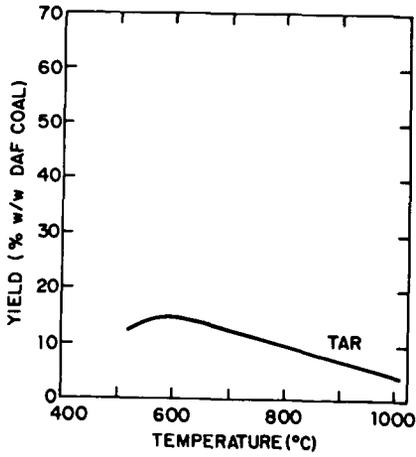


FIGURE 3  
 PYROLYSIS OF TEXAS LIGNITE  
 YIELDS OF PRINCIPAL GASES

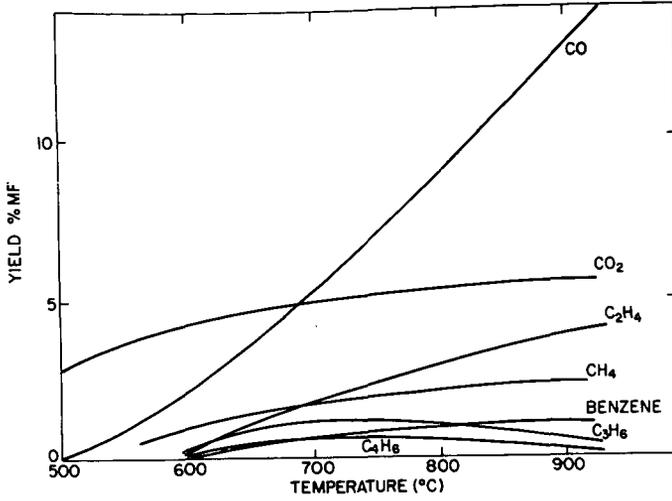
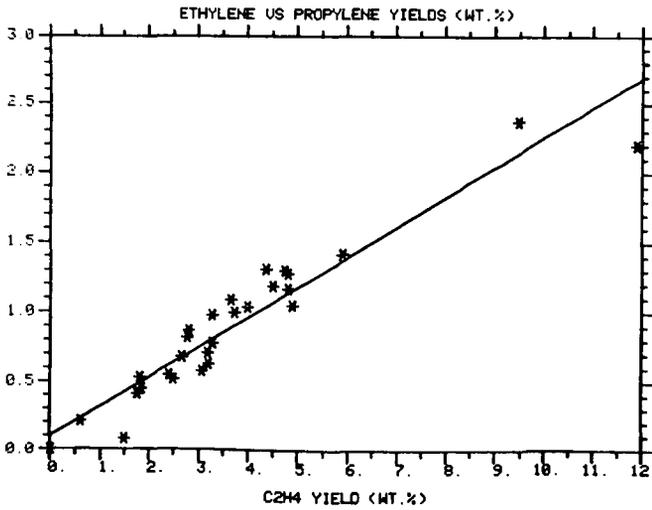


FIGURE 4

C<sub>3</sub>H<sub>6</sub> (WT. %)

14:56 16-JAN-83



C2H4 YLD (WT. %)

FIGURE 6

08:19 8-MAR-63

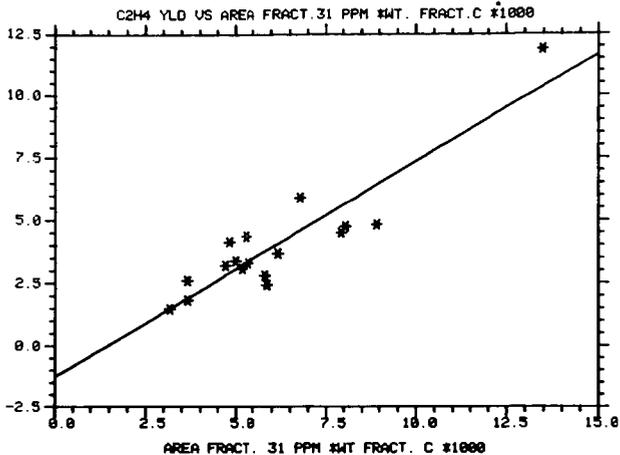


FIGURE 5  
<sup>13</sup>C NMR SPECTRA OF COALS PRODUCING DIFFERENT ETHYLENE YIELDS ON PYROLYSIS (850°C 4sec. CT)

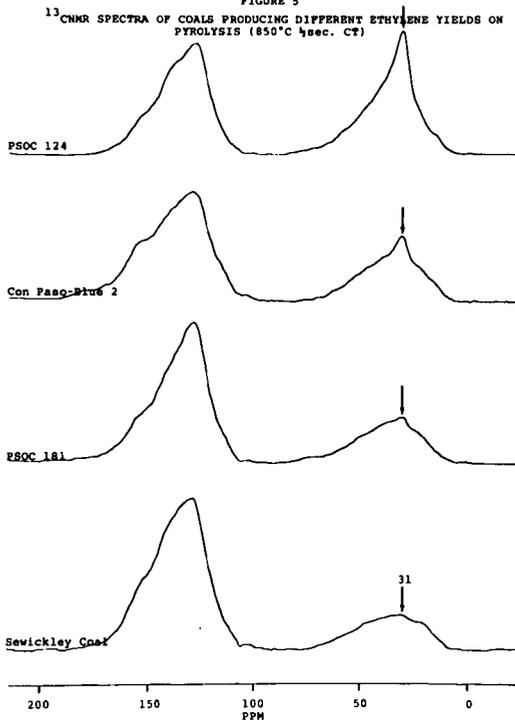




FIGURE 9

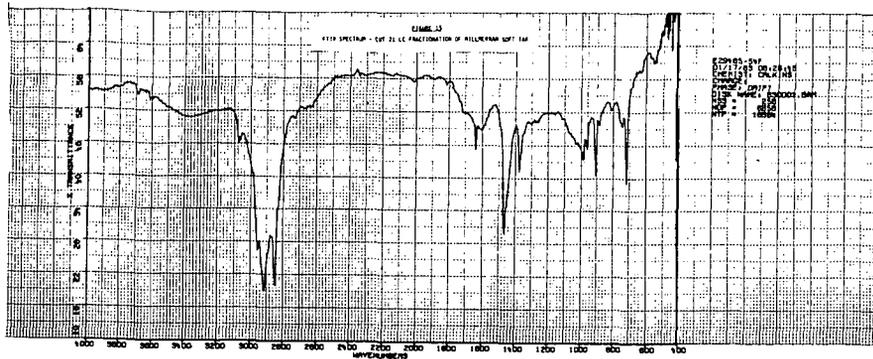


FIGURE 10

GC/MS SPECTRUM - CUT 21 LC FRACTIONATION OF MILLERRAN SOFT TAR

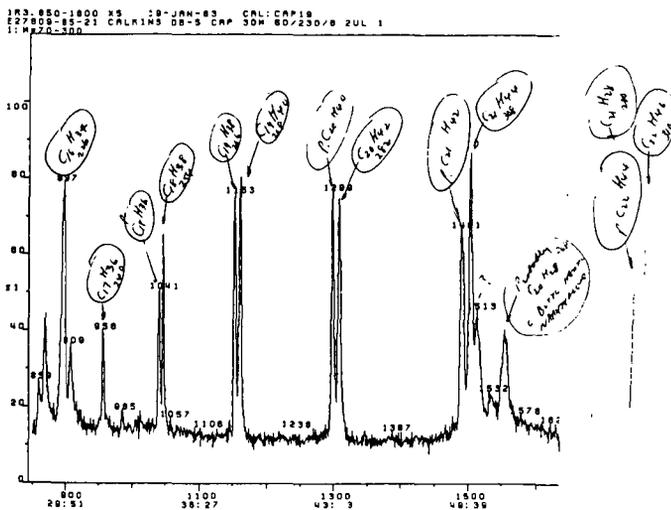




TABLE 1

ETHYLENE YIELDS IN COAL PYROLYSIS AND (CH<sub>2</sub>)<sub>n</sub> CONTENT (WT. %)

(850°C 0.5 sec. CT.)

<u>Coal</u>	<u>MF*</u>	<u>MAF**</u>	<u>(CH<sub>2</sub>)<sub>n</sub> (MF)*</u>
PSOC 124	11.9	13.1	17.0
King Cannel	9.47	11.04	14.5
Millmerran	6.08	7.01	9.65
Lovelady-L-2	5.91	7.94	9.11
Lovelady Y-4	4.90	6.68	8.40
Lovelady 81 VLL-92	4.82	7.00	8.48
Blind Canyon	4.82	5.07	6.56
PSOC 435	4.75	4.98	8.86
Emery	4.50	4.95	7.12
Con Paso-Blue 3	4.36	4.88	5.72
Con Paso-Blue 2	3.73	4.78	7.21
Con Paso-Yellow 4	3.67	4.17	5.18
Upper Hiawatha	3.30	3.65	5.03
Wyodak	3.21	3.52	4.0
<u>Texas Lignite</u>	3.20	3.59	6.01
PSOC 181	3.07	3.33	5.02
Con Paso-Yellow 6	2.80	3.05	4.31
PSOC 464	2.78	3.06	4.12
Lower Hiawatha	2.66	2.85	5.00
Pittsburgh 8	2.50	2.98	4.47
PSOC 1106	2.42	2.53	4.04
PSOC 657	1.85	2.28	2.18
Illinois 6-Burning Star	1.83	2.18	1.75
PSOC 833	1.77	2.01	2.00
Sewickley	1.48	1.75	2.20
Ohio 9-Egypt Valley	.61	.68	1.78
Anthracite	0.0	0.0	0.0

\*Moisture Free

\*\*Moisture and Ash Free

TABLE 2

(CH<sub>2</sub>)<sub>n</sub> ANALYSIS OF KNOWN COMPOUNDS  
(Proton NMR)

	<u>Theory</u>	<u>Found</u>
CH <sub>3</sub> [(CH <sub>2</sub> ) <sub>14</sub> ]CH <sub>2</sub> CH <sub>2</sub> - $\overset{\text{O}}{\underset{\text{  }}{\text{C}}}$ -OH	64.0	62.6
CH <sub>3</sub> [(CH <sub>2</sub> ) <sub>10</sub> ]CH <sub>3</sub>	82.0	77.7
CH <sub>3</sub> [(CH <sub>2</sub> ) <sub>13</sub> ]CH <sub>3</sub>	85.8	81.8
CH <sub>3</sub> [(CH <sub>2</sub> ) <sub>17</sub> ]CH <sub>3</sub>	88.8	84.6
CH <sub>3</sub> [(CH <sub>2</sub> ) <sub>22</sub> ]CH <sub>3</sub>	91.1	91.7
CH <sub>3</sub> [(CH <sub>2</sub> ) <sub>23</sub> ]CH <sub>3</sub>	91.5	92.5
 CH <sub>2</sub> CH <sub>2</sub> [(CH <sub>2</sub> ) <sub>9</sub> ]CH <sub>3</sub>	51.2	49.1

TABLE 3

600°C. PYROLYSIS TARS - DISTRIBUTION OF TYPES OF H ATOMS

PPM	0.8	1.3	1.6-1.7	1.7-3.0	5.2	7.2
H TYPE	CH <sub>3</sub>	(CH <sub>2</sub> ) <sub>n</sub>		hydroaromatic or benzylic	olefinic	aromatic
<u>COAL TYPE</u>						
Texas Lignite	.085	.352	.077	.300	--	.187
Emery	.099	.331	.064	.263	.016	.232
PSOC 124	.110	.349	.170	.190	.010	.175
PSOC 435	.113	.220	.113	.267	.003	.166

TABLE 4

PYROLYSIS TARS - DISTRIBUTION OF H ATOMS  
TEXAS LIGNITE PYROLYSIS VS. TEMPERATURE

H TYPE	PPM	.3 - .5	.8	1.3	1.6 - 1.7	1.7 - 3.0	5.2	6.5 - 8.0
			CH <sub>3</sub>	(CH <sub>2</sub> ) <sub>N</sub>		HYDROAROMATIC	OLEFINIC	AROMATIC
600		=	.110	.320	.048	.259	.044	.141
700		=	.100	.254	.036	.258	.048	.250
825		=	.067	.189	.027	.208	.053	.414
850		.009	.035	.078	.106	.159	.009	.566
920		.027	.018	.099	.117	.072	-	.577

TABLE 5

PYROLYSIS OF MODEL COMPOUNDS (LIQUIDS)  
 (0.3 ml/hr Liquid Feed in ca 2.1 l/min. N<sub>2</sub>)  
 850°C 0.5-1.0 Sec. Contact Time

<u>Model Compound</u>	<u>Gaseous or Volatile Products</u>	
	<u>Principal Products</u>	<u>Minor Products</u>
Stearic Acid	C <sub>2</sub> H <sub>4</sub> C <sub>3</sub> H <sub>6</sub> C <sub>4</sub> H <sub>6</sub> CH <sub>4</sub> CO <sub>2</sub>	Benzene C <sub>2</sub> H <sub>6</sub>
Dodecane	C <sub>2</sub> H <sub>4</sub> C <sub>3</sub> H <sub>6</sub> CH <sub>4</sub>	C <sub>4</sub> H <sub>6</sub> C <sub>2</sub> H <sub>6</sub>
Octadecane	C <sub>2</sub> H <sub>4</sub> CH <sub>4</sub> C <sub>3</sub> H <sub>6</sub>	C <sub>4</sub> H <sub>6</sub> C <sub>2</sub> H <sub>6</sub>
Ethyl Benzene	Styrene Toluene Methane	C <sub>2</sub> H <sub>6</sub> Benzene C <sub>2</sub> H <sub>4</sub>
Propyl Benzene	Toluene Ethylene Styrene	Benzene Methane Ethyl Benzene
n-Butyl Benzene	Ethylene Toluene Ethyl Benzene Methane Styrene	C <sub>2</sub> H <sub>6</sub> C <sub>3</sub> H <sub>6</sub> Benzene
Phenyl Dodecane	Ethylene Propylene Methane Toluene Styrene	C <sub>4</sub> H <sub>6</sub> C <sub>2</sub> H <sub>6</sub> Benzene

TABLE 6

ESTIMATES OF  $(CH_2)_N$  IN COAL (WT.%)

COAL	COAL FROM		FROM 600°C		FROM COAL	
	YIELDS	PYROLYSIS	PYROLYSIS TAR	LIQUEFACTIONS(MACRO)2000 PSI H <sub>2</sub>	(NA <sub>2</sub> S, FESO <sub>4</sub> CATALYSTS) *	
	%C <sub>2</sub> H <sub>4</sub> 850°C	C <sub>2</sub> H <sub>4</sub> plus other hydro- carbons	% $(CH_2)_N$	TEMPERATURE 925°C/2 hrs	TIME	YIELD
PITTSBURGH 8	2.5	4.2	-	2.38	1.91	4.10 4.36 5.2
TEXAS LIGNITE	3.2	5.3	3.3	5.49	-	6.59 6.45
WYODAK	3.21	5.3	-	-	4.84	5.06 6.42
EMERY	4.5	7.5	5.2	7.77	-	8.77 7.3 8.60
PSOC 435	4.75	7.9	3.5	9.02	8.39	9.57 7.14 7.39
MILLMERRAN	6.10	10.2	4.4	-	-	9.65 12.35
PSOC 124	11.90	17.3	9.2	16.47	17.6	13.9 16.4 17.7

\* ASSUMES 100% CONVERSION OF ORGANIC PORTION

\*\* LOW CONVERSION, VERY VISCOUS PRODUCT

\*\*\* DIHYDROPHENANTHRENE

\*\*\*\* TETRAHYDROQUINOLINE

TABLE 7

COAL LIQUEFACTION ANALYSIS FOR (CH<sub>2</sub>)<sub>n</sub> IN COAL (WT.%)

<u>Coal</u>	<u>Liquefactions(Micro) 425°C/2 hr.</u>			<u>Liquefactions(Macro) 2000 psi H<sub>2</sub></u>	
	<u>Tetralin</u>	<u>DHP</u>	<u>IHQ</u>	<u>IHQ</u>	<u>425°C/2 hr.</u>
Pittsburgh 8	1.81	1.72	4.63	4.36	
Texas Lignite	3.07	3.88	6.02	6.59	
Wyodak			6.3	5.06	
Emery	6.99	-	7.12	7.3	
PSOC 435	4.82	5.19	7.73	7.14	
Millmerran	4.31	6.57	9.13	9.65	
PSOC 124	9.02	9.32	16.58	16.4	