/   /

(NJC)

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. α   .2

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Abstract

Determination of the Octane Number for many commercial gasolines samples of a known octane number and authentic aromatic was carried out. Aromatic hydrocarbons were added to improve the octane number. Calculation depend on the multiparametric regrestional analysis, parameters and the experimental determination of protons from NMR spectra, symmetry in the system, nature of the mixture and aniline point. The study revealed that, octane number is affected directly by:

1. Aromatic proton in mono cyclic aromatics.
2. Proton content in α-position and higher protons.
3. Monocyclic Naphthenic proton contents.
4. Octane number decrease by increasing chain length of the substituent attached to aromatic system.
5. Method of blending gasoline.

(9,10).

(2,2,4-Tri methyl Pentane)

(n-C$_7$H$_{16}$)   .

(10).   %10

                                                                                                          (1).

(4 , 9 , 10)(RON).   (2).

                    (6-8)(MON).   (3).

        (GLC,IR ,NMR)

                                                                                                          (4,5).

                                        .

            (10-14).   (6,7).

)

                        :

                                        .   (8)(.

    (15).

                                        .

                                                                              (9).

            (15,16)().

                                1500

.   .

(17)   (15)

3. **NMR** :

(NMR)

(PIONA)   ^{1}HNMR

Hitachi-Perkin Elmer

Spectrophotometer (R24-B) 60 MHz   .
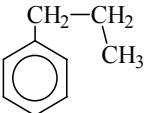
. (etc…, Hme, Hmy, Hα, Ha)

4.   :

(5,12-16)

(5 , 4 , 3 , 2)

1.   :

.

[N]   [S]   )

5.   :

(

(2)

(2)

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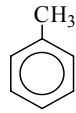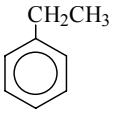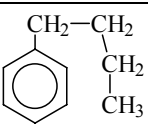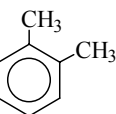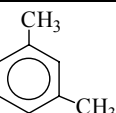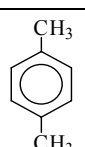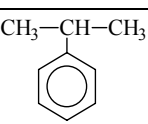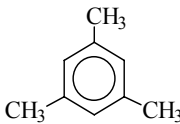
2.   :

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NMR

(7)

(1)   .

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:(**1**)

Compound	Structure	ON Prac	ON The.	نقطة الإنيلان	Ha	Hx	Hn	Hmy	Hm	S	Nature
Benzene	(benzene ring)	99	106.339	19	100	0	0	0	0	1	0
	CH₃ (toluene)	124	118.411	21	83.33	16.66	0	0	0	0	0
	CH₂CH₃ (ethylbenzene)	124	128.675	22	71.42	14.28	0	0	14.2	0	0
	CH₂—CH₂ CH₃ (propylbenzene)	127	108.067	23	62.5	12.5	0	12.5	12.5	0	0
	CH₂—CH₂ CH₂ CH₃ (butylbenzene)	98	91.172	25	55.55	11.11	0	22.22	11.11	0	0
	_	77	79.829	26	31.25	12.5	0	37.5	18.75	0	0
	_	60	66.440	27	27.77	11.11	0	44.44	16.66	0	0
	CH₃ CH₃ (o-xylene)	120	135.381	27	66.66	33.33	0	0	0	0	0
	CH₃ CH₃ (m-xylene)	145	141.974	28	66.66	33.33	0	0	0	1	0
	CH₃ CH₃ (p-xylene)	146	141.687	28.5	66.66	33.33	0	0	0	1	0
	CH₃—CH—CH₃ (cumene)	132	135.993	24	62.5	12.5	0	0	25	0	0
	CH₃ CH₃ CH₃ (mesitylene)	171	169.033	25	33.33	33.33	0	0	33.33	0	0
	_	81	76.825	36	24.59	11.51	13.26	30.96	19.66	0	1
	_	83	85.941	32	16.55	5.72	12.18	31.25	34.28	0	1
	_	88	88.776	29	21.81	10.94	14.52	28.06	24.65	0	1
	_	91	91.684	27	22.32	6.913	19.11	23.69	26.95	0	1
	_	78	97.764	25	23.42	11.47	21.18	21.54	22.36	0	1

(Hme)   .9

.   (1)

(Hmy)   .10   :

.   .1

(S)   .11   .

.   .2

(Nature)   .12   .

(ON)   .3

.

(ON)   .4

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.5

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(Ha)   .6

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.(2)   (Hα)   .7

.   α

(HN)   .8

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:**(2)**

Point	Ha	Hx	Hn	Hmy	Hm	S	Nature	ON The.	ON Prac.
19.0	100.0	0.000	0.00	0.00	0.00	1	0	106.339	99
21.0	83.33	16.66	0.00	0.00	0.00	0	0	118.411	124
22.0	71.42	14.28	0.00	0.00	14.20	0	0	128.675	124
23.0	62.50	12.50	0.00	12.50	12.50	0	0	108.067	127
25.0	55.55	11.11	0.00	22.22	11.11	0	0	91.172	98
26.0	31.25	12.50	0.00	37.50	18.75	0	0	79.829	77
27.0	27.77	11.11	0.00	44.44	16.66	0	0	66.440	60
27.0	66.66	33.33	0.00	0.00	0.00	0	0	135.381	120
28.0	66.66	33.33	0.00	0.00	0.00	1	0	141.974	145
28.5	66.66	33.33	0.00	0.00	0.00	1	0	141.687	146
24.0	62.50	12.50	0.00	0.00	25.00	0	0	135.993	132
25.0	33.33	33.33	0.00	0.00	33.33	0	0	169.033	171
36.0	24.59	11.51	13.26	30.96	19.66	0	1	76.825	81
32.0	16.55	5.720	12.18	31.25	34.28	0	1	85.941	83
29.0	21.81	10.95	14.52	28.06	24.65	0	1	88.776	88
27.0	22.32	6.913	19.11	23.69	26.95	0	1	91.684	91
25.0	23.42	11.47	21.18	21.54	22.36	0	1	97.764	78

.(1)
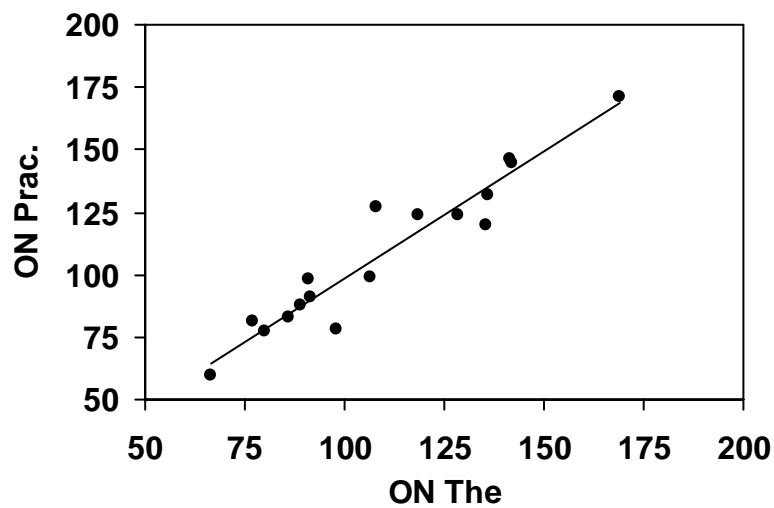
:(1)

.(1)

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:

The regression equation is:

ON = - 0.57 Point + 1.10 Ha + 2.32
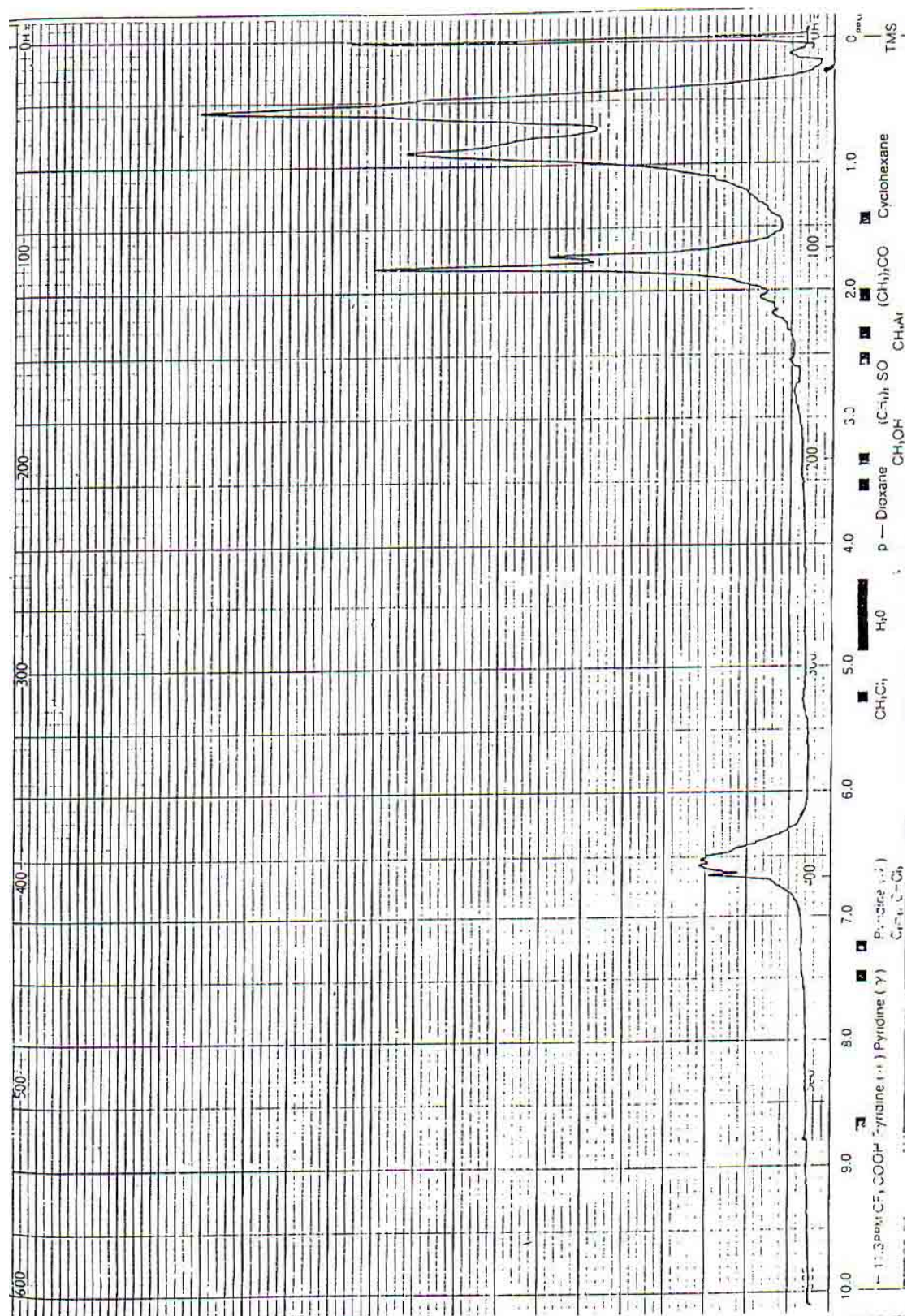Hα + 1.07 Hn – 0.204 Hmy +
      2.08 Hm + 7.17 S – 5.1 Nat

.

:(2)

:(3)

:(4)
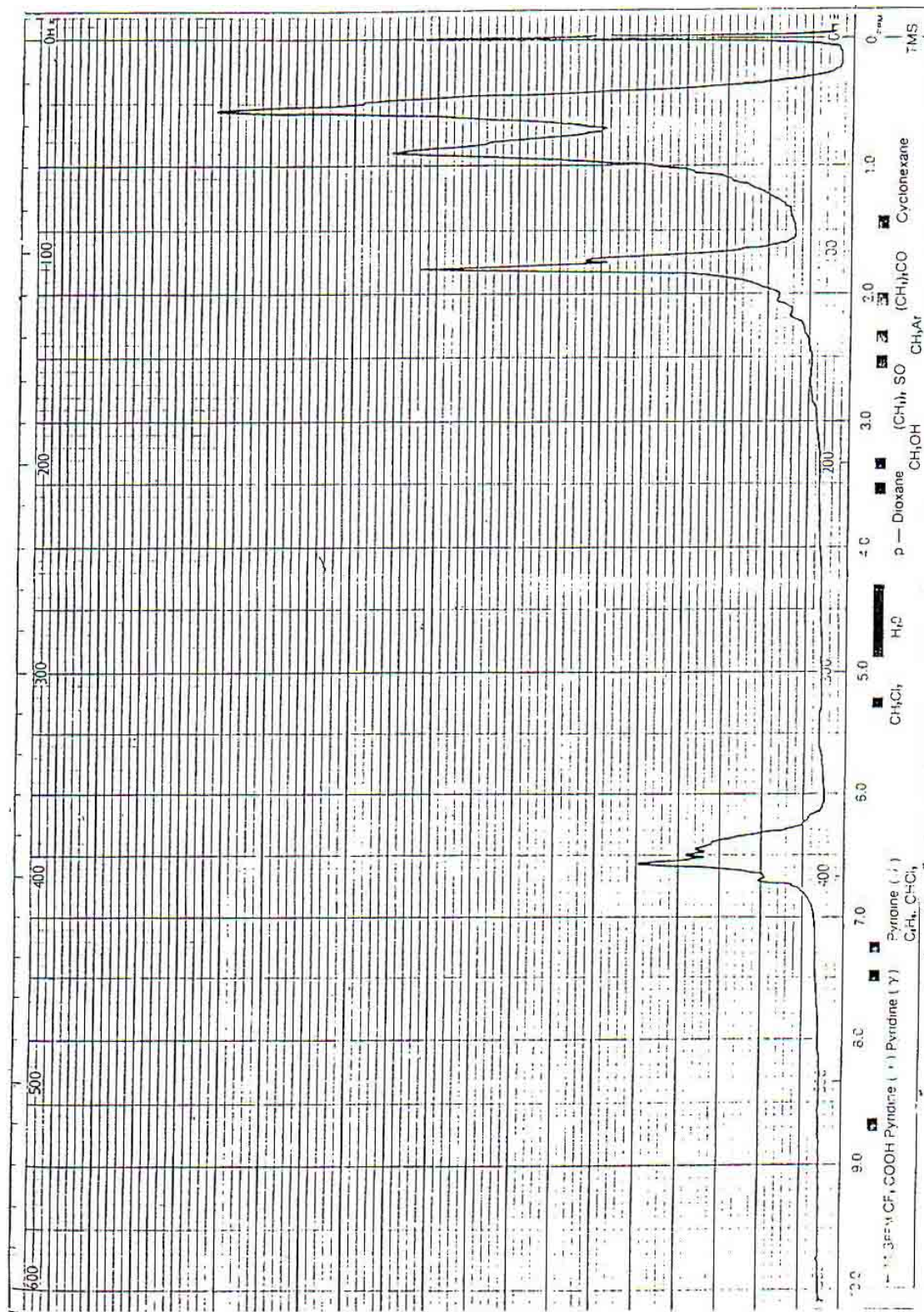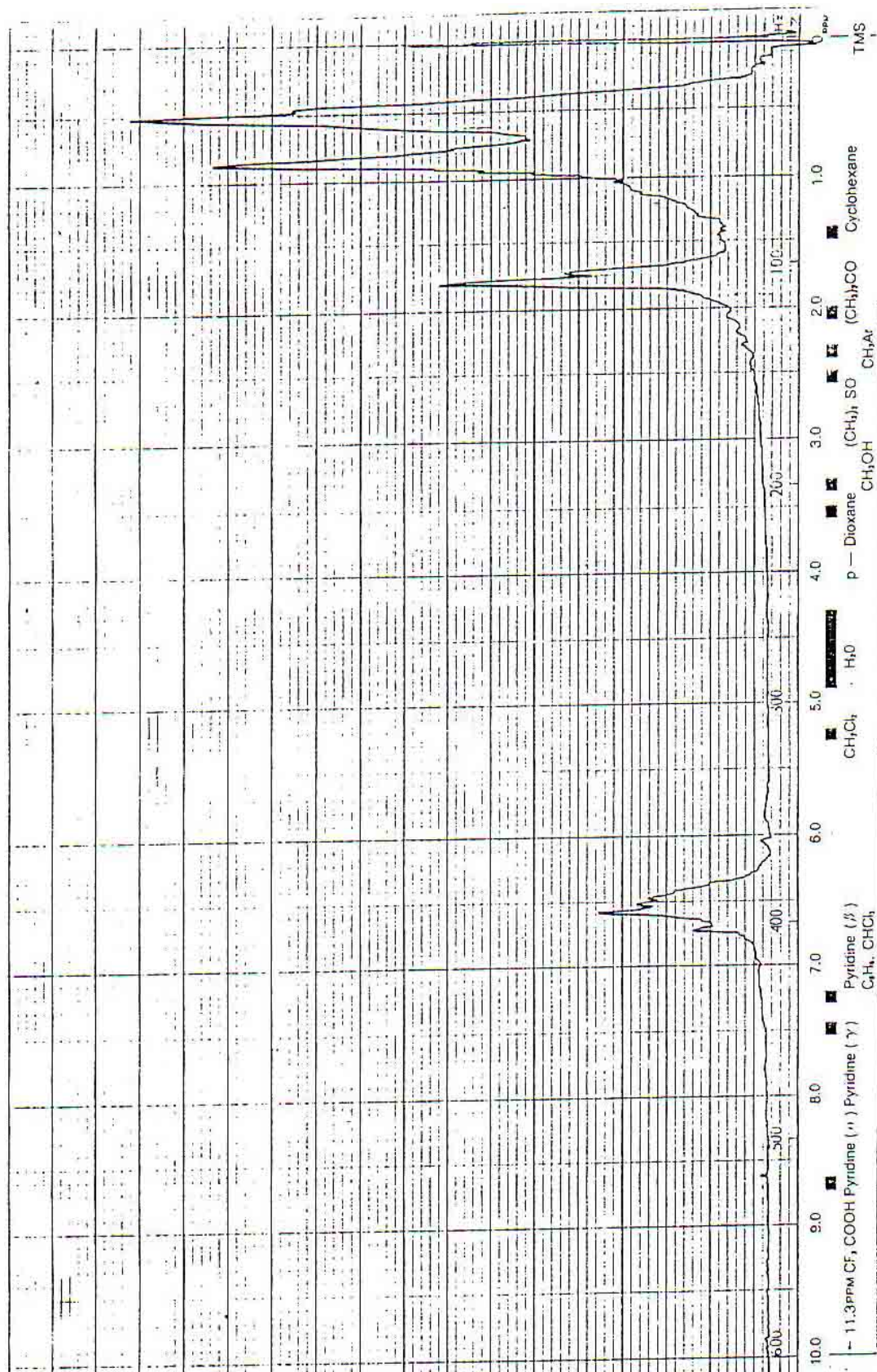
:(5)

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