

TITLE PAGE

13. Verbindungen in den leichten
Fraktionen des Steinkohlenteeres.
Compounds contained in the
light fractions of bituminous
coal tar.

Frame Nos. 286 - 304

Verbindungen in den leichten Fraktionen

13

des Steinkohlenteeres.

I. Hochtemperaturteer.

Das Leichtöl des Hochtemperaturteeres (80-170° siedend), das 2-3 % des Rohteeres ausmacht, enthält:

Phenole	5-15 %
Basen	1-3 %
S-haltige Stoffe	0,1 %
O-haltige neutrale Stoffe	0,2-0,3 %
Kohlenwasserstoffe	<u>81,6-93,7 %</u>
	100,00 %.

Von diesen rund 80 % aromatischen Kohlenwasserstoffen entfallen auf Benzol, Toluol und Xylole 64 %.

Die Xylolfraktion
des Teeres enthält:

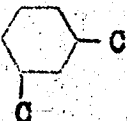
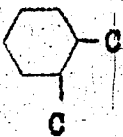
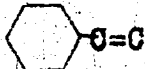
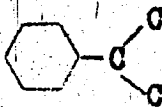
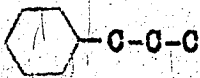
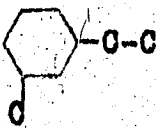
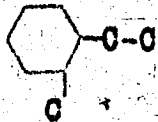
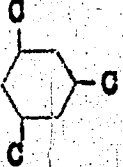
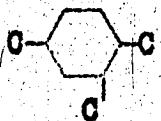
Zum Vergleich
Xylolfraktion aus Erdöl:

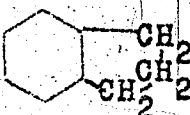
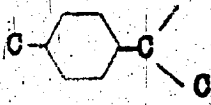
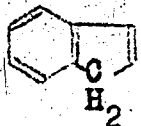
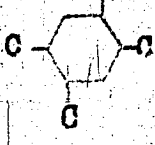
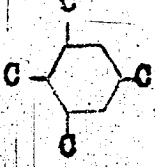
m-Xylol	68-70 %	36-38 %
o-Xylol	3-5 %	7-9 %
p-Xylol	18-19 %	12-13 %

An leichtersiedenden Verbindungen -200°C wurden in dem Hochtemperaturteer nachgewiesen:

1. Aromatische Kohlenwasserstoffe:

Verbindung	Formel	Sdp. °C
Benzol		80,2
Toluol		111

Verbindung	Formel	Sdp. °C
Äthylbenzol		136
p-Xylol		138,5
m-Xylol		139
o-Xylol		142,3
Styrol		145
Isopropylbenzol		153
n-Propylbenzol		159
p-Äthyltoluol		161,2
m-Äthyltoluol		162
o-Äthyltoluol		164,5
Mesitylen		165
Pseudocumol		168

Verbindung	Formel	Sdp. °C
Hemellitol		175
Hydrinden		176
Cymol		177
Inden		182,3
Durol		190
Isodurol		195,7
Methylinden		195-200

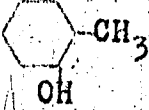
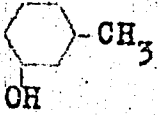
2. Naphthene.

Verbindung	Formel	Sdp. °C
Cyklopentadien	$\begin{array}{c} \text{C}=\text{C} \\ \quad \diagup \\ \text{C}=\text{C} \quad \text{C} \end{array}$	41
Cyklohexan	$\begin{array}{c} \text{C}-\text{C} \\ / \quad \backslash \\ \text{C} \quad \text{C} \\ \backslash \quad / \\ \text{C}-\text{C} \end{array}$	80,8
Cyklohexen	$\begin{array}{c} \text{C}=\text{C} \\ / \quad \backslash \\ \text{C} \quad \text{C} \\ \backslash \quad / \\ \text{C}-\text{C} \end{array}$	83,0
Cyklohexadien	C_6H_8	84
Methyloxylohexan	$\begin{array}{c} \text{C}-\text{C} \\ / \quad \backslash \\ \text{C} \quad \text{C} \\ \backslash \quad / \\ \text{C}-\text{C} \end{array}$	101
Dimethyloxylohexan	C_8H_{16}	118

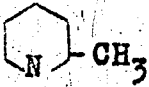
3. Olefine und Diolefine.

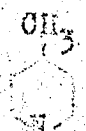
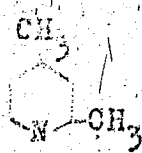
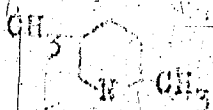
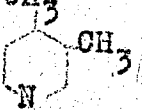
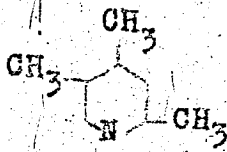
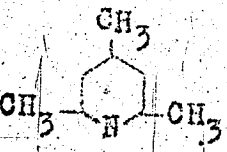
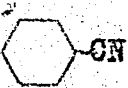
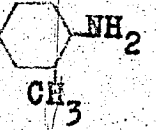
Verbindung	Formel	Sdp. °C
1,3-Butadien	$\text{C}=\text{C}-\text{C}=\text{C}$	1
Crotonylen	$\text{C}-\text{C}=\text{C}-\text{C}$	28
Amylen	C_5H_{10}	40
Hexylen	C_6H_{12}	69
Heptylen	C_7H_{14}	98

4. Sauerstoffhaltige Verbindungen.

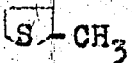
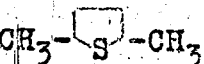
Verbindung	Formel	Sdp. °C
Aceton	$\text{CH}_3 \cdot \text{CO} \cdot \text{CH}_3$	80
Cumaron		174
Phenol		181
o-Kresol		191
Methylcumaron		190-195
p-Kresol		201,8
m-Kresol		202,8

5. Stickstoffhaltige Verbindungen.

Verbindung	Formel	Sdp. °C
Acetonitril	CH_3CN	79
Pyridin		115
2-Methylpyridin		129
Pyrrol		131
3-Methylpyridin		143

Verbindung	Formel	Sdp. °C
2,6-Dimethylpyridin		143
4-Methylpyridin		145
2,4-Dimethylpyridin		157
2,5- " "		163
2,3- " "		164
3,4- " "		164
2,4,5-Trimethylpyridin		167
2,4,6- " "		171
Anilin		184
Benzonitril		196
o-Toluidin		200

6. Schwefelhaltige Verbindungen.

Verbindung	Formel	Sdp. °C
Methylmercaptan	$\text{CH}_3 \cdot \text{SH}$	6
Äthylmercaptan	$\text{CH}_3 \cdot \text{CH}_2 \cdot \text{SH}$	37
Dimethylsulfid	$\text{CH}_3 \cdot \text{S} \cdot \text{CH}_3$	37,5
Schwefelkohlenstoff	CS_2	47
Thiophen		84
Diäthylsulfid	$\text{CH}_3 \cdot \text{CH}_2 \cdot \text{S} \cdot \text{CH}_2 \cdot \text{CH}_3$	92
1-Methylthiophen		113
1,4-Dimethylthiophen		137

II.

Tieftemperatur-Teer.

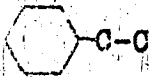
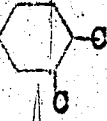
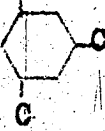
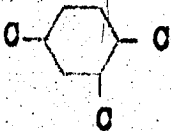
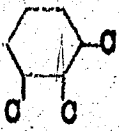
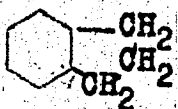
Die leicht siedenden Fraktionen des Steinkohlentief-
temperaturteeres enthalten an gesättigten und an aromatischen
Verbindungen folgende Mengen:

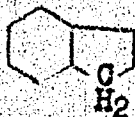
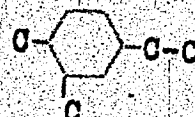
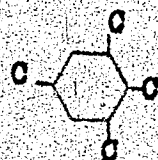
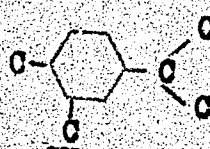
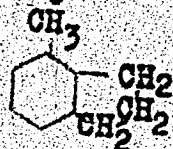
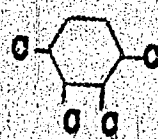
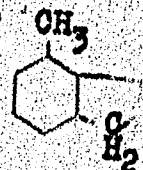
Fraktion °C	Gesättigte Verbin- dungen %	Aromatische Ver- bindungen %
30-78	29	0
78-85	25	0
85-90	28	0
90-100	21	0
100-105	16	0
105-110	10	3
110-115	14	6
115-120	12	0
120-125	28	0
125-130	18	0
130-135	10	24
135-140	23	15
140-145	24	21
145-150	27	7
150-155	14	-
155-160	18	-

Von diesen aromatischen Verbindungen sind bezogen
auf Leichtöl:

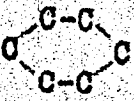
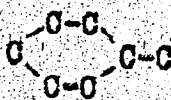
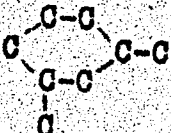
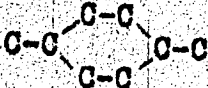
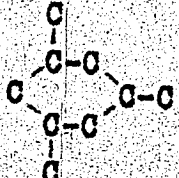
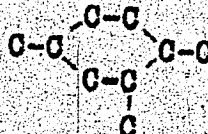
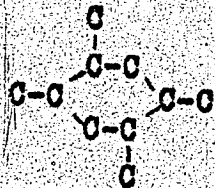
Benzol 4-5,9 %
Toluol und Xylol 2-2,5 %

In den leichten Fraktionen -200°C des Steinkohlentief-
temperaturteeres wurden folgende Verbindungen nachgewiesen:
1. Aromatische Verbindungen.

Verbindung	Formel	Sdp. $^{\circ}\text{C}$
Benzol		80,2
Toluol		111
Äthylbenzol		136
Dihydro-m-xylol	C_8H_{12}	137
p-Xylol		138,5
o-Xylol		142,3
p-Äthyltoluol		161,2
Dihydrotrimethyl- benzol	C_9H_{14}	164
Mesitylen		165
Pseudocumol		168
Dihydromesitylen	C_9H_{14}	168
Dekalin	$\text{C}_{10}\text{H}_{18}$	169,5
Hemellitol		175
Hydrinden		176

Verbindung	Formel	Sdp. °C
Dihydroprehnitol	$C_{10}H_{16}$	182
Inden		182,3
3,4-Dimethyläthylbenzol		189
Isodurool		195,7
1,2-Dimethyl-4-isopropylbenzol		199
4-Methylhydrinden		203
Prehnitol		204
4-Methylinden		205

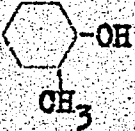
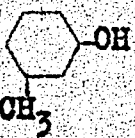
2. Naphthene.

Verbindung	Formel	Sdp. °C
Cyklopentadien		41
Cyklohexan		80,8
Methylcyklohexan		101
1,3-Dimethyl- cyklohexan		118
1,4- " "		123
1,3,5-Trimethyl- cyklohexan		137
1,2,4- " "		143
1,2,4,5-Tetramethyl- cyklohexan		174

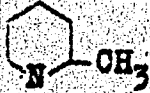
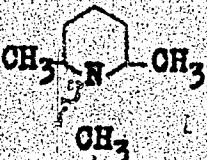
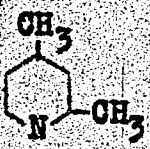
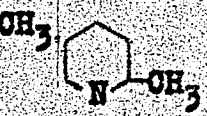
3. Olefine.

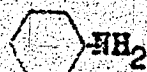
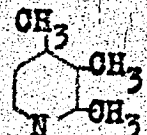
Verbindung	Formel	Sdp. °C
Pentilen-(1)	$C=C-C-C-C$	40
Oktylen	C_8H_{16}	126
Nonylen	C_9H_{18}	150
Undecylen	$C_{10}H_{20}$	190

4. Sauerstoffhaltige Verbindungen.

Verbindung	Formel	Sdp. °C
Phenol		181
o-Kresol		191
p-Kresol		201,8
m-Kresol		202,8

5. Stickstoffhaltige Verbindungen.

Verbindung	Formel	Sdp. °C
Pyridin		115
1-Methylpyridin		129
2,6-Dimethylpyridin		143
4-Methylpyridin		145
2,4-Dimethyl-		157
2,5- " "		163

Verbindung	Formel	Sdp. °C
2.3.6-Trimethylpyridin		174
Anilin		184
2.3.5-Trimethylpyridin		185
2.3.4- " "		188
Toluidin		200

6. Schwefelhaltige Verbindungen.

Verbindung	Formel	Sdp. °C
Methylmercaptan	$\text{CH}_3 \cdot \text{SH}$	6
Dimethylsulfid	$\text{CH}_3 - \text{S} - \text{CH}_3$	37,5

gez. Henkels

Literatur:

Heydenreich, Die deutsche Steinkohlenteerindustrie und ihre wirtschaftlichen Zusammenhänge.

Kruber, Angw. Chem. 53, 69

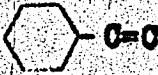
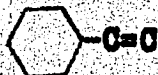
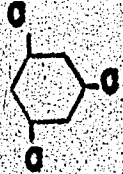
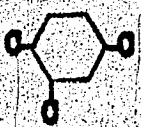
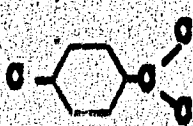
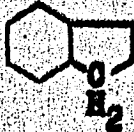
Stadnikoff, Die Chemie der Kohlen.

Klein, Brennstoffchemie 2, 3.

Verbindungen aus gekracktem Erdöl.

In den leichten Fraktionen -200°C von gekracktem Erdöl wurden folgende Verbindungen nachgewiesen:

1. Aromatische Kohlenwasserstoffe.

Verbindung	Formel	Sdp. $^{\circ}\text{C}$
Benzol		80
Toluol		111
Xylole	3 Isomere	138-144
Phenylacetylen		141
Styrol		146
Mesitylen		164
Pseudocumol		169
Cymol		176
Index		182

2. Naphthene.

Verbindung	Formel	Sdp. °C
a) Fünfringe		
Cyklopentadien	$\begin{array}{c} \text{C}=\text{C} \\ \quad \diagup \\ \text{C}=\text{C} \quad \text{C} \end{array}$	42
Methyloyklopentan	$\begin{array}{c} \text{C}-\text{C} \\ \quad \diagup \\ \text{C}-\text{C} \quad \text{C} \end{array}$	71,8
Methyloyklopentadien	C_6H_8	72,8
Dimethyloyklopentan	C_7H_{14}	
b) Sechseringe		
Cyklohexan	$\begin{array}{c} \text{O}-\text{O}-\text{O} \\ \diagdown \quad \diagup \\ \text{O} \quad \text{O}-\text{O} \quad \text{O} \end{array}$	80,8
Methyloyklohexan	$\begin{array}{c} \text{O}-\text{O}-\text{O} \\ \diagdown \quad \diagup \\ \text{O} \quad \text{O}-\text{O} \quad \text{O}-\text{O} \end{array}$	100,8

3. Olefine.

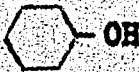
In den leichten Fraktionen des gekraackten Erdöls finden sich Gemische von einfach ungesättigten Isomeren mit 5-10 C-Atomen.

An mehrfach ungesättigten Verbindungen wurden ermittelt:

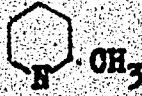
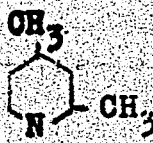
Verbindung	Formel	Sdp. °C
Diacetylen	$\text{C} \equiv \text{C}-\text{C} \equiv \text{C}$	10,3
Isopren	$\text{C}=\text{C}-\text{C}=\text{C}$	32
1-Methylbutadien	$\text{C}-\text{C}=\text{C}-\text{C}=\text{C}$	43
Hexadien	Isomerengemische	-

- 3 -

4. Sauerstoffhaltige Verbindungen.

Verbindung	Formel	Sdp. °C
a) Carbonsäuren		
Ameisensäure	HCO_2H	100,7
Essigsäure	$\text{CH}_3 \cdot \text{CO}_2\text{H}$	118,2
Propionsäure	$\text{CH}_3 \cdot \text{CH}_2 \cdot \text{CO}_2\text{H}$	141,4
Buttersäure	$\text{CH}_3\text{CH}_2 \cdot \text{CH}_2 \cdot \text{CO}_2\text{H}$	164
n-Valeriansäure	$\text{CH}_3 \cdot \text{CH}_2 \cdot \text{CH}_2 \cdot \text{CH}_2 \cdot \text{CO}_2\text{H}$	187
Isovaleriansäure	$\begin{array}{c} \text{CH}_3 \\ \text{CH}_3 \end{array} \text{OH} \text{CH}_2 \text{CO}_2\text{H}$	176,5
n-Capronsäure	$\text{CH}_3 \cdot \text{CH}_2 \cdot \text{CH}_2 \cdot \text{CH}_2 \cdot \text{CH}_2 \cdot \text{CO}_2\text{H}$	202
b) Phenole		
Phenol		182
Kresole	3 Isomere	190-202

5. Stickstoffhaltige Verbindungen.

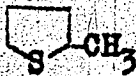
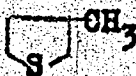
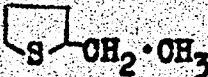
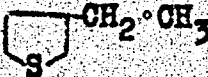
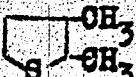
Verbindung	Formel	Sdp. °C
2-Methylpyridin		129
2,6-Dimethylpyridin		142
4-Methylpyridin		144
2,4-Dimethylpyridin		157,8
2,5- " "		160
3,5- " "		170

Schwefelhaltige Verbindungen.

Verbindung	Formel	Sdp. °C
a) Aliphatische Verbindungen		
Äthylmercaptan	$\text{CH}_3 \cdot \text{CH}_2 \cdot \text{SH}$	34,5
Methylsulfid	$\text{CH}_3 - \text{S} - \text{CH}_3$	36
Isopropylmercaptan	$\begin{array}{c} \text{CH}_3 \\ \text{CH}_3 \end{array} \text{CH} \cdot \text{SH}$	52,4
Methyläthylsulfid	$\text{CH}_3 - \text{S} - \text{CH}_2 - \text{CH}_3$	66
Isobutylmercaptan	$\begin{array}{c} \text{CH}_3 \\ \text{CH}_3 \end{array} \text{CH} \cdot \text{CH}_2 \cdot \text{SH}$	88
Äthylsulfid	$\text{CH}_3 \cdot \text{CH}_2 \cdot \text{S} - \text{CH}_2 \cdot \text{CH}_3$	92
Äthylpropylsulfid	$\text{C}_2\text{H}_5 - \text{S} - \text{C}_3\text{H}_7$	116
Amylmercaptan	$\text{C}_5\text{H}_{11} \cdot \text{SH}$	130
n-Propylsulfid	$\text{C}_3\text{H}_7 - \text{S} - \text{C}_3\text{H}_7$	142
Heptylmercaptan	$\text{C}_7\text{H}_{15} \cdot \text{SH}$	176-178
n-Butylsulfid	$\text{C}_4\text{H}_9 \cdot \text{S} - \text{C}_4\text{H}_9$	182
Oktylmercaptan	$\text{C}_8\text{H}_{17} \cdot \text{SH}$	201-204

und weitere aliphatische Sulfide mit Gruppen bis zu 6 C-Atomen.

b) Cyclische Verbindungen

Verbindung	Formel	Sdp. °C
Thiophen		84
α -Methylthiophen		113
β -Methylthiophen		114
2-Ethylthiophen		133
3- " "		136
2,3-Dimethylthiophen		137
3,4- " "		145

ges. Henkels

Literatur:

Waldmann, Erdölbestandteile.

Tetrahedron
Zusammenfassung: Aromatische Kohlenwasserstoffe in den Benzing
fraktionen (bis 200°) aus Erdöl, gekrackten Erdöl, Steinkohl-
hoch- und tieftemperaturteer.

Verbindung	Sdp.	Erdöl		Steinkohlenteer	
			gekrackt	Hochtemp.	Tieftemp.
Benzol	80,2°	+	+	+	+
Toluol	111°	+	+	+	+
Äthylbenzol	136°	-	-	+	+
p - Xylol	138,5°	+	+	+	+
m - Xylol	139°	+	+	+	-
Phenylacetylen	141°		+	-	-
o - Xylol	142,3°	+	+	+	+
Styrol	145°	-	+	+	-
Isopropylbenzol	153°	-	-	+	-
n-Propylbenzol	159°	-	-	+	-
p-Äthyltoluol	161,2°	}	-	+	+
m-Äthyltoluol	162°		-	+	-
o-Äthyltoluol	164,5°		-	+	-
Mesitylen	165°	-	+	+	+
Pseudocumol	168°	+	-	+	+
Hemellitol	175°	+	-	+	+
m - Cymol	176°	+	-	-	-
Hydrinden	176°	-	-	+	+
Cymol	177°	+	+	+	-
Inden	182,3°	-	+	+	+
3,4-Dimethyläthylbenzol	189°	-	-	-	+
Isocamylbenzol	189-194°	+	-	-	-
Durool	190°	+	-	+	-
Diäthylbenzol	190-195°	+	-	-	-
Isodurool	195,7°	+	-	+	-
1,2-Dimethyl-4-isopropylbenzol	199°	-	-	-	+
Methylinden	200°	-	-	+	-
Diäthyltoluol	200°	+	-	-	-
4 Methylhydrinden	203°	-	-	-	+
Prehnitol	204°	+	-	-	+
4-Methyl-inden	205°	-	-	-	+

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