TABLE II

SUMMARY OF CALCULATED VALUES USING EQUATION (6) AND OF EXPERIMENTAL DATA

	$K_M \times 10^5$ HAc		$K_M \times 10^5$ HB		$K_M \times 10^{11}$ H_2Q		$K_M \times 10^3$ ClHAc	
F_D	Exptl.[6]	Calcd.	Exptl.[7]	Calcd.	Exptl.[7]	Calcd.	Exptl.[8]	Calcd.
0.0	1.84	(1.84)	6.09	(6.09)	2.66	(2.66)	1.73	(1.73)
9.61					2.35			
25.18					1.94			
26.40		1.36		4.60		1.81		1.37
28.4	1.352							
48.4	1.088							
51.45			3.56					
52.42			3.55					
54.69					1.30			
55.60		0.988		3.41		1.23		1.05
77.1	0.741							
77.49					0.889			
78.49		.756		2.61		0.895		0.827
87.99			2.23					
92.51		.622		2.18		.722		.700
93.0	.608							
96.00					(.684)			
96.51			2.03					
97.0	.575							
97.87			1.99					
98.67					.657			
100	(.555)	(.555)	(1.95)	(1.95)	(.639)	(.639)	(0.631)	(.631)

The K_M values, calculated from the revised equation (6), are now in very good agreement with the experimental results. These are summarized in Table II and plotted in Figs. 1, 2, and 3. The predicted slope for chloroacetic acid is given in Fig. 4; no experimental data for comparison are available. The value of K_D for salicylic acid is extrapolated with equation (6) from the average value $K_M = 0.24 \times 10^{-3}$, a. d. 12%, at $F_D = 91.7$, and from the average $K_H = 0.98 \times 10^{-3}$, a. d. 2%, determined by Korman and La Mer.[1] The K_D thus calculated is 0.21×10^{-3} which also has not yet been determined experimentally.

It is apparent that true values of hydrogen and deuterium ion concentrations are obtainable from kinetic data when tested by means of acid dissociation constants.

(6) (Acetic acid) Chittum and La Mer, THIS JOURNAL, **59**, 2524 (1937).

(7) (Benzoic acid and hydroquinone) Rule and La Mer, *ibid.*, **60**, 1974 (1938).

(8) (Chloroacetic acid) Lewis and Schultz, *ibid.*, **56**, 1913 (1934).

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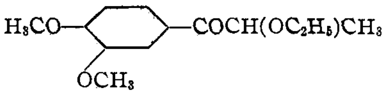
The Structure of Lignin

BY A. B. CRAMER, M. J. HUNTER AND HAROLD HIBBERT

In a recent note[1] the isolation of a new aromatic ketone ($C_{13}H_{18}O_4$) was described. This has now been identified (by direct synthesis and mixed melting point determination) as α-ethoxypropioveratrone



The synthesis (after numerous unsuccessful attempts, and using a variety of methods) was accomplished as follows:

$$\begin{tikzcd}[column sep=small]
 & \text{Veratrole} + \text{propionyl chloride} \arrow[r] & \text{Propioveratrone} \arrow[r] & {} \\
\alpha\text{-Brompropioveratrone} \arrow[rr] & & \text{Acetate of } \alpha\text{-hydroxypropioveratrone} \arrow[dl] \arrow[dr] & \\
 & \alpha\text{-Hydroxypropioveratrone} \arrow[rr] & & \alpha\text{-Ethoxypropioveratrone}
\end{tikzcd}$$

The synthetic compound melted at 81–82°; a mixed melting point with natural compound gave no depression. The melting point of the 2,4-dinitrophenylhydrazone of the natural compound is 134–136°; synthetic compound, 134–136°; the mixed melting point also showed no depression.

(1) Cramer, Hunter and Hibbert, THIS JOURNAL, **60**, 2274 (1938).

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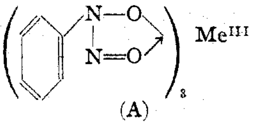
The Classification of Chelating Groups

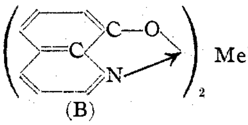
BY HELMUT M. HAENDLER AND BRADFORD P. GEYER

In the course of preliminary work on organic analytical reagents which form inner complex compounds with metal ions, it was found advisable to devise a system for the classification of chelating groups present in various organic compounds to serve as a basis of comparison. The available classifications, in particular that of Diehl,[1] are too unwieldy for rapid grouping and comparison. In addition to classifying the organic compounds now known, any system should also present information concerning possible reagents. The common method of indicating the number of members in the completed chelate ring is too cumbersome, in view of the recent increases in both number and variety of compounds possessing groups capable of chelation.

TABLE I

Group designation	Representative compound
C-N, SH	Mercaptobenzothiazole
C-NH, SH	Rubianic acid
C-NOH, OH	Benzohydroxamic acid
N-NONH$_4$, O	Cupferron (A)
C,C-N, NOH	Phenyl α-pyridyl ketoxime
C,C-N, OH	8-Quinolinol (B)
C,C-N, SH	8-Quinolinethiol
C,C-NH, SH	Thionalide
C,C-NH$_2$, OH	Glycocoll
C,C-NOH, NOH	Dimethylglyoxime (C)
C,C-NOH, O	α-Nitroso-β-naphthol
C,C-O, OH	Oxalic acid
C,C-O, SH	Thioglycolic acid
C,C-OH, OH	Catechol
C,C-OH, S	Thiohydantoic acid
C,N-NH, NOH	Nitrosoguanidine
C,N-NH$_2$, OH	Hydrazinecarboxylic acid
C,N-NH$_2$, SH	Dithizone (D)
C,C,C-N, NH	Chlorophyll type
C,C,C-NOH, OH	Salicylaldoxime (E)
C,C,C-O, OH	Alizarin
C,C,N-N, NH	Phthalocyanine
C,C,N-NH, NH	Biguanidine
C,C,N-NH, NH$_2$	Biuret
C,C,N-NH, O	Dicyandiamidine (F)


(A)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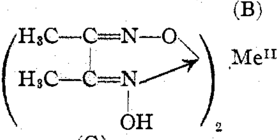
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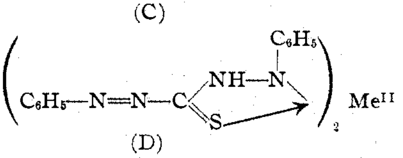
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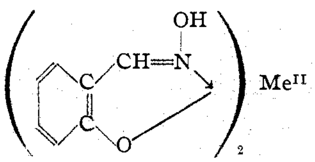
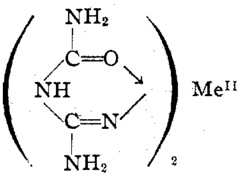

(E)


(F)

In this classification the two functioning groups, which supply the primary and secondary valences involved in the general formation of a chelate ring, and the atom or atoms linking these two groups form the basis of the system. Compounds with identical chelating groups have the same group designation, regardless of the structure of the remainder of the molecule. The group designation is derived as follows: (*a*) The atom or atoms connecting the two functional groups are expressed by their conventional symbols, arranged alphabetically. (*b*) The functioning groups are given by their symbolic representations in alphabetical order of the atoms by which they are attached to the original compound before chelation.

In salicylaldoxime, for example, the functional groups are linked by three carbon atoms, and these functional groups are the oxime and hydroxyl radicals. Consequently, the classification is C,C,C-NOH, OH.

The accompanying list gives in order of increasing complexity the designations of the more common chelating groups and the names of representative compounds containing such groupings. For the sake of clarity, structural formulas illustrating some of the inner complexes formed are also given. It is evident that exact knowledge of the structure of the chelate compound formed is not essential for this method, insofar as the primary and secondary valence connections are concerned. No attempt is made to designate these linkages as to type, and compounds are arranged solely on the basis of general structure.

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[1] H. Diehl, *Chem. Rev.*, **21**, 39-111 (1937).

Dynamic Isomerism of Acetaldehyde 2,4-Dinitrophenylhydrazone

BY W. M. D. BRYANT

In earlier papers the writer[1,2] presented conclusive evidence based on optical crystallographic measurements that there are at least two distinct crystalline modifications of acetaldehyde 2,4-

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[1] Bryant, THIS JOURNAL, **55**, 3201 (1933).

[2] *Ibid.*, **58**, 2335 (1936).