[CONTRIBUTION FROM THE DEPARTMENT OF CHEMISTRY, UNIVERSITY OF TEXAS]

The Number of Structural Isomers of the More Important Types of Aliphatic Compounds[1]

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It has been shown that, by separating the isomers of each specified carbon atom content into types, arbitrarily chosen upon the basis of their structural formulas and deriving mathematical formulas of the (finite) recursion type for each, it is possible to calculate the total number of structural isomers of the methanol, paraffin, ethylene, and acetylene series.[2] The method has been extended to include all of the more important types of aliphatic compounds and the numbers of structural isomers of such compounds are indicated in the following tables.[3]

TABLE I

NUMBER OF STRUCTURAL ISOMERS

Aliphatic type	No. of isomers	Aliphatic type	No. of isomers
Acetals	*a*	Disubstituted paraffins	
Acids		$C_NH_{2N}XY$	*h*
monocarboxylic	*b*	$C_NH_{2N}X_2$	*i*
dicarboxylic	*c*	Esters	*f*
amino	*d*	Ethers	*j*
hydroxy	*d*	Glycols	*k*
sulfinic	*e*	Isonitriles	*b*
sulfonic	*e*	Ketones	*l*
Aldehydes	*b*	Mercaptans	*e*
Alkyl halides	*e*	Nitriles	*b*
Amides		Quaternary ammonium compounds	*m*
unsubstituted	*b*	Sulfones	*j*
monosubstituted	*f*	Sulfoxides	*j*
disubstituted	*a*	Thioethers	*j*
Amines		Thioureas	*n*
primary	*g*	Ureas	*n*
secondary	*g*		
tertiary	*g*		

[a] Equal in number to that of Group C of the ethylenes of $N + 1$ carbon content, THIS JOURNAL, **55**, 681–682 (1933).[4] [b] Equal to the number of methanols of $N - 1$ carbon content. [c] Equal to the number of disubstitution products of the paraffins containing two identical substituents, $C_NH_{2N}X_2$, of $N - 2$ carbon content, see Table II. [d] Equal to the number of disubstitution products of the paraffins containing two unlike substituents, $C_NH_{2N}XY$, of $N - 1$ carbon content, see Table II; the number of structurally isomeric alpha amino or hydroxy acids is equal to the number of acetylenes of the same carbon content. [e] Equal to the number of methanols of the same carbon content. [f] Equal to the number of esters of the same carbon content, see Table II. [g] The numbers of p., s. and t. amines are equal to the numbers of p., s. and t. methanols, respectively, of $N + 1$ carbon content. [h] See Table II. [i] See Table II. [j] Equal to the number of secondary methanols of $N + 1$ carbon content. The "simple" ethers equal the methanols of $N/2$ carbon content. [k] See Table II. [l] Equal to the number of secondary methanols of same carbon content; the number of methyl ketones is equal to that of the methanols of $N - 2$ carbon content. [m] See Table II. [n] Equal to the number of ethylenes of $N + 1$ carbon content.

TABLE II

Carbon content	No. of esters	Number of quaternary ammonium compounds	No. of glycols	No. of disubstituted paraffins Type $C_NH_{2N}XY$	Type $C_{2N}H_NX_2$
1				1	1
2	1		1	2	2
3	2		2	5	4
4	4	1	6	12	9
5	9	1	14	31	21
6	20	3	38	80	52
7	45	7	97	210	129
8	105	18	260	555	332
9	249	42	688	1479	859
10	599	109	1856	3959	2261
15	57,564	11,733	273,824	576,221	312,246
20	6,589,734	1,451,178	42,599,485	88,594,746	46,972,357

Summary

The structural isomerism of the more important types of aliphatic compounds has been considered and for each of these types the numbers of structural isomers, for certain carbon atom contents, have been calculated.

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(1) Abstracted from Part II of the doctoral dissertation of Charles M. Blair, University of Texas, June, 1933.

(2) Henze and Blair, THIS JOURNAL, **53**, 3042, 3077 (1931); **55**, 680 (1933); Coffman, and Blair with Henze, *ibid.*, **55**, 252 (1933).

(3) The various formulas from which the calculations of the numbers of structural isomers were made, together with the necessary theoretical foundations for the same, appear in Chapters II–IV of Part II of the dissertation on file in the University of Texas Library.

(4) Mr. Julian M. Mavity has called to our attention that the number of structurally isomeric tetradecylenes reported on page 685 under Group C, type (2) as being 200 should be corrected to read 100. Hence the total number of structural isomers of $C_{14}H_{27}$ is 14,397.