

SECTION OF ANALYTICAL CHEMISTRY  
COMMISSION ON MICROCHEMICAL TECHNIQUES\*

RECOMMENDED TEST SUBSTANCES FOR THE  
MICRODETERMINATION OF CARBON  
AND HYDROGEN

A number of compounds are recommended for use as test substances for the microdetermination of carbon and hydrogen in organic substances. All of these substances, or a proper selection from the list, may be used to determine the universal applicability of a given method, either already described or one which might be developed in the future.

The compounds selected are stable over long periods of time and are non-hygroscopic (any exceptions to the latter generalization are noted). The substances are either commercially available in a sufficiently pure state to be used for tests based on the accuracy of present-day methods, or may be purified or prepared by conventional laboratory means to meet these standards.

The compounds selected include the following:

- (1) those which have extreme values (high as well as low) for carbon and/or hydrogen contents;
- (2) compounds representing a variety of structural types;
- (3) compounds containing elements which may cause interferences in the carbon-hydrogen determination.

These recommendations may be changed or supplemented as the need arises.

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	Empirical formula	Molecular weight	C (%)	H (%)	O (%)	N (%)	Hal (%)	S (%)	Element (%)
C, H									
Anthracene	$C_{14}H_{10}$	178.234	94.34	5.66					
Cyclohexane	$C_6H_{12}$	84.162	85.63	14.37					
Naphthalene	$C_{10}H_8$	128.174	93.71	6.29					
O (C, H)									
Benzoic acid	$C_7H_6O_2$	122.125	68.85	4.95	26.20				
Cholesterol	$C_{27}H_{46}O$	386.665	83.87	11.99	4.14				
d-Glucose (dextrose)	$C_6H_{12}O_6$	180.162	40.00	6.71	53.29				
Phthalic acid anhydride	$C_8H_6O_3$	148.120	64.87	2.72	32.41				
Stearic acid	$C_{18}H_{36}O_2$	284.486	76.00	12.76	11.25				
N (C, H, O)									
Acetanilide	$C_8H_9ON$	135.168	71.09	6.71	11.84	10.36			
Caffeine (1,3,7-trimethyl-xanthine anhydrous)	$C_8H_{10}O_2N_4$	194.200	49.48	5.19	16.48	28.85			
2,4-Dinitrophenylhydrazine	$C_6H_6O_4N_4$	198.146	36.37	3.05	32.30	28.28			
Diphenylamine	$C_{12}H_{11}N$	169.228	85.17	6.55		8.28			
Hexamethylenetetramine	$C_6H_{12}N_4$	140.194	51.40	8.63		39.97			
Picric acid	$C_6H_3O_7N_3$	229.114	31.45	1.32	48.88	18.34			
F (C, H, O, . . .)									
<i>p</i> -Fluorobenzoic acid	$C_7H_5O_2F$	140.117	60.00	3.60	22.84		F (%)		
Perfluorodicyclohexylethane	$C_{12}F_{26}$	662.154	25.39				13.56		
Trifluoroacetamide	$C_8H_6ONF_3$	189.144	50.80	3.20	8.46	7.41	74.61		
Cl (C, H, . . .)									
Chloroacetamide	$C_2H_4ONCl$	93.519	25.69	4.31	17.11	14.98	37.91		
1-Chloro-2,4-dinitrobenzene	$C_6H_3O_4N_2Cl$	202.563	35.58	1.49	31.60	13.83	17.50		
Hexachlorobenzene	$C_6Cl_6$	284.808	25.30				74.70		
Hexachlorocyclohexane	$C_6H_6Cl_6$	290.856	24.78	2.08			73.14		
Tetrachloro- <i>p</i> -benzoquinone (chloranil, tetrachloroquinone)	$C_6O_2Cl_4$	245.894	29.31		13.01		57.68		
Br (C, H, . . .)									
<i>p</i> -Bromoacetanilide	$C_8H_8ONBr$	214.076	44.88	3.77	7.47	6.54	37.33		
2,4,6-Tribromophenol	$C_6H_3OBr_3$	330.838	21.78	0.91	4.84		72.47		

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I (C, H, ...)	Erythrosin (iodoosin, 2,4,5,7-tetraiodofluorescein)	C <sub>20</sub> H <sub>8</sub> O <sub>3</sub> I <sub>4</sub>	835.924	28.74	0.96	9.57	I (%) 60.73	As (%) 34.51
S (C, H, ...)	S-Benzylthiuronium chloride Sulphanilamide Sulphanilic acid (anhydrous) Sulphonal Thiourea	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub> I	248.027	33.90	2.03	12.90	51.17	P (%) 8.99
		C <sub>8</sub> H <sub>11</sub> N <sub>2</sub> ClS	202.715	47.40	5.47	13.82	Cl (%) 17.49	11.81
		C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> N <sub>2</sub> S	172.212	41.85	4.68	16.27	15.82	Ca (%) 31.29
		C <sub>8</sub> H <sub>7</sub> O <sub>3</sub> N <sub>2</sub> S	173.196	41.61	4.07	18.58	18.62	Hg (%) 59.57
		C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	228.337	36.82	7.06	27.71	18.51	K (%) 19.15
	76.125	15.78	5.30	28.03	28.09	Na (%) 34.31	42.12	
P, As (C, H, ...)	o-Arsanilic acid (o-aminophenylarsonic acid)	C <sub>6</sub> H <sub>8</sub> O <sub>3</sub> NaS	217.048	33.20	3.72	22.11	6.45	
5-Chloro-4-hydroxy-3-methoxy-benzylisothiourae phosphate* Triphenylphosphine		C <sub>9</sub> H <sub>14</sub> O <sub>6</sub> N <sub>2</sub> ClSP	344.725	31.36	4.09	27.85	10.29	
		C <sub>18</sub> H <sub>15</sub> P	262.293	82.43	5.76	8.13	9.30	
Me (C, H, ...)	Calcium oxalate	C <sub>2</sub> O <sub>4</sub> Ca	128.102	18.75		49.96		
Phenylmercuric acetate		C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> Hg	336.762	28.53	2.39	9.50		
		C <sub>3</sub> H <sub>5</sub> O <sub>1</sub> K	204.228	47.05	2.47	31.34		
Potassium acid phthalate		C <sub>2</sub> O <sub>4</sub> Na <sub>2</sub>	134.004	17.93		47.76		

\* W. H. Smith. *Anal. Chem.*, 30, 149 (1958).**Notes**

For the calculation of molecular weights and percentages, the atomic weights used are those proposed by the Commission on Atomic Weights of the I.U.P.A.C., 1957.

The percentage figures are given to the second decimal. Where the third decimal is less than 0.005, the last figure has been disregarded. Where the last figure has been rounded off, it has been underlined (0.375 = 0.38).