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USE OF MODERN INSTRUMENTS IN THE CHEMISTRY CLASS OF HIGH SCHOOL

——UV AND IR SPECTROMETERS, pH-METERS, AND MICROCOMPUTERS

YOSHIHISA OTANI
University of Tsukuba Senior High School
at Komaba

Summary

Modern instruments are used in various fields of chemistry. These instruments are useful in teaching high school students in chemistry:

1. Students understand modern methods of studying chemistry.
2. They not only actively study chemistry but also are positively involved in various kinds of experiments in chemistry.
3. They can easily understand several subjects in the field of chemistry.

Examples of Use

1. UV-Spectrometers

1-a. Chemical Kinetics

Phenolpthalein, methylviolet, and malakaitgreen have colors in week alkali solutions, but they change carbinol types and become colorless in strong alkali solutions. Fig. 1 is an example of them. (phenolphthalein)

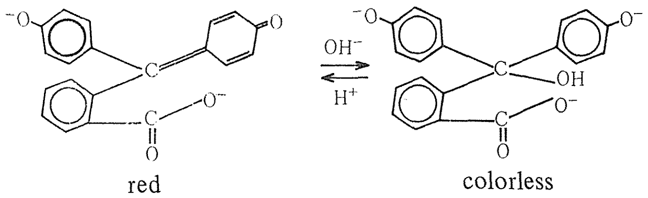


Fig. 1 Phenolphthalein

If the concentrations of dyes is shown as C, the velocities of fading follows the next equation.

$$-\frac{dC}{dt} = kC\,[\,OH^-\,] \qquad \cdots\cdots \quad (1)$$

In large quantities of $[OH^-]$, the equation can be considered first-order. Or $[OH^-]$ can be considered constant.

$$-\ln C = k[\,OH^-\,]\,t + \mathrm{const} \qquad \cdots\cdots \quad (2)$$

By Beer's law

$$C = K \cdot A \qquad (A\text{: Absorption}) \qquad \cdots\cdots \quad (3)$$

And the initial concentration Co is equivalent to "const".

$$-\ln KA = k[\,OH^-\,]\,t - \ln Co \qquad \cdots\cdots \quad (4)$$

$$\log A = \log \frac{Co}{K} - \frac{k[OH^-]}{2.303}\,t \qquad \cdots\cdots \quad (5)$$

Absorption is related to time, and the equation is first-order. So if absorption and $[OH^-]$ are measured, then k will be calculated. This is an useful experiment for teaching chemical kinetics in high school.

Examples of experimental data by students are Fig. 2 and Table 1. Concentrations of dyes are $10^{-6} \sim 10^{-5}$ mol/ℓ, and temperatures are $20 \sim 25$°C. $[OH^-]$ is determined with the titration of oxalic acid.

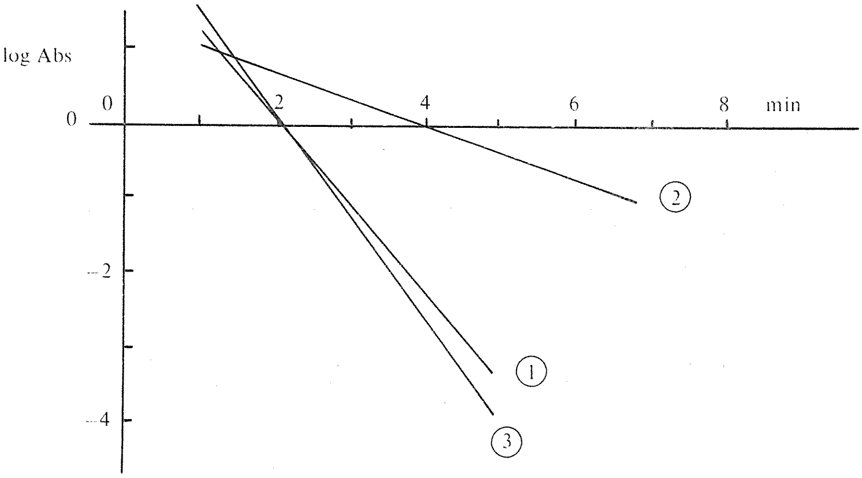


Fig. 2 ① Phenolphthalein ② Methylviolet ③ Malakaitgreen

Table 1

	Wave length (nm)	Slope	$[OH^-]$	k (min^{-1})
phenolphthalein	550	0.130	0.595	1.00
methylviolet	590	0.00175	0.0175	8.95
malakaitgreen	610	0.13	0.0096	62.4

$$k = \frac{\text{slope} \times 2.303}{[OH^-] \times \frac{1}{2}}$$

1-b. Equilibrium Constant

5 mℓ of 2.0×10^{-5} mol/ℓ $Fe_2(NO_3)_3$ is added to various kinds of concentration of KSCN- 0.5×10^{-3} mol/ℓ, 1.0×10^{-3} mol/ℓ, 2×10^{-3} mol/ℓ, 3.0×10^{-3} mol/ℓ. And absorptions of mixed solutions are measured with spectrometer in 460 nm.

$$Fe^{3+} + SCN^{-} \rightleftharpoons FeSCN^{2+}$$

The calibration curve of $FeSCN^{2+}$ is Fig. 3. Examples of students' data are Table 2.

Table 2

	initial $[Fe^{3+}]$ $\times 10^{-4}$	initial $[SCN^{-}]$ $\times 10^{-4}$	absorption 460 nm	$[FeSCN^{2+}]$ $\times 10^{-4}$	mixed $[Fe^{3+}]$ $\times 10^{-4}$	mixed $[SCN^{-}]$ $\times 10^{-4}$	K (460 nm)
①	9.671	2.56	0.21	0.45	9.226	2.12	228
②		5.12	0.435	0.92	8.749	4.20	251
③		10.24	0.85	1.8	7.871	8.44	271
④		15.36	1.22	2.6	7.071	12.76	2.88

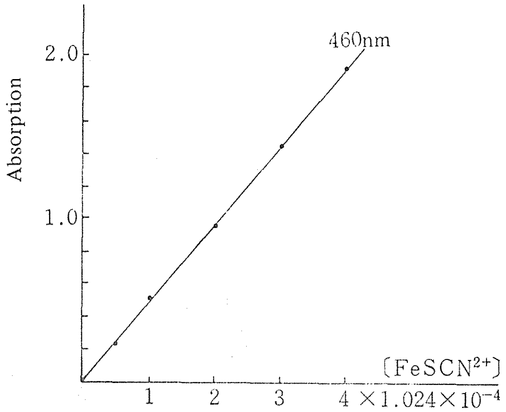


Fig. 3 Calibration Curve

$[FeSCN^{2+}]$ can be found from absorption data, and $[Fe^{3+}]$ and $[SCN^{-}]$ can be calculated with $[FeSCN^{2+}]$. So the values of equilibrium constant K are calculated with the next equations.

$$K = \frac{[Fe\,SCN^{2+}]}{[Fe^{3+}]\,[SCN^{-}]} \quad \cdots\cdots\cdots\cdots \quad (6)$$

1-c. Aquation of Praceosalt

Dissolved trans- $Co(en)_2Cl_2Cl$ changes to be cis-form and its Cl^- is explaced with OH^-. This change can be observed with measuring the spectrum from 400 to 800 nm. Initial green color changes to be gray and becomes red finally.

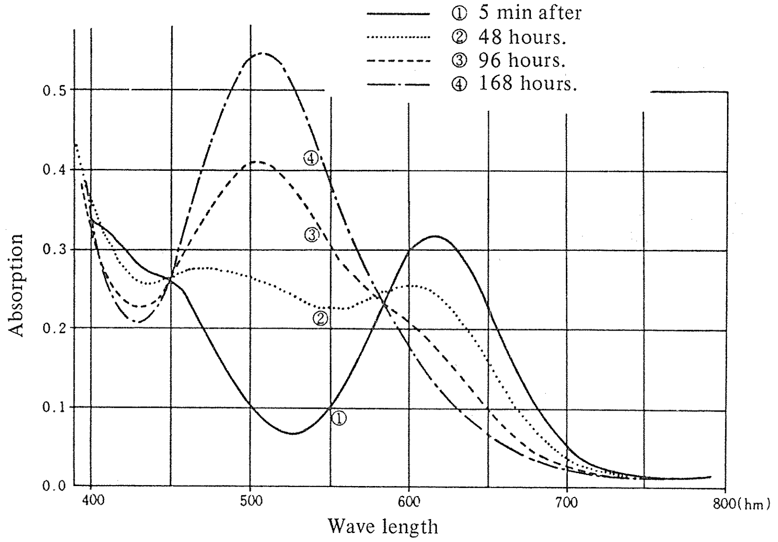


Fig. 4 Spectrums of $Co(en)_2C\ell_2C\ell$

2. IR-Spectrometers

2-a. Synthesys and Measuring

Students synthesize nitrobenzene, aniline, acetanilide and acetate-esters, and take IR-spectrums of the compounds.

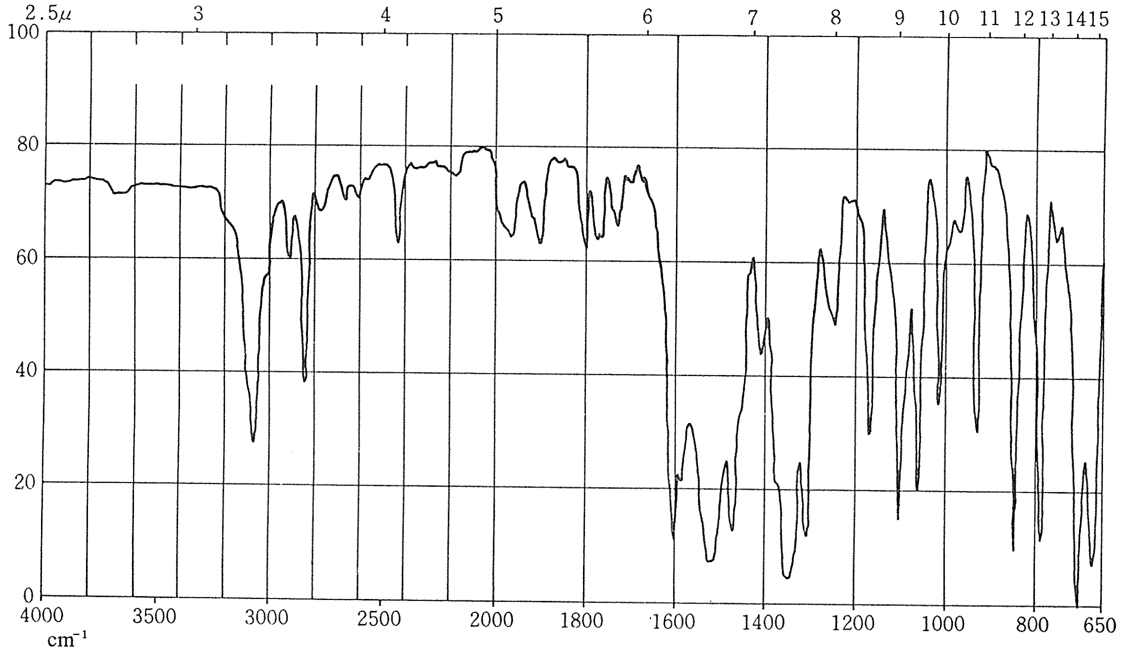


Fig. 5 Nitrobenzene

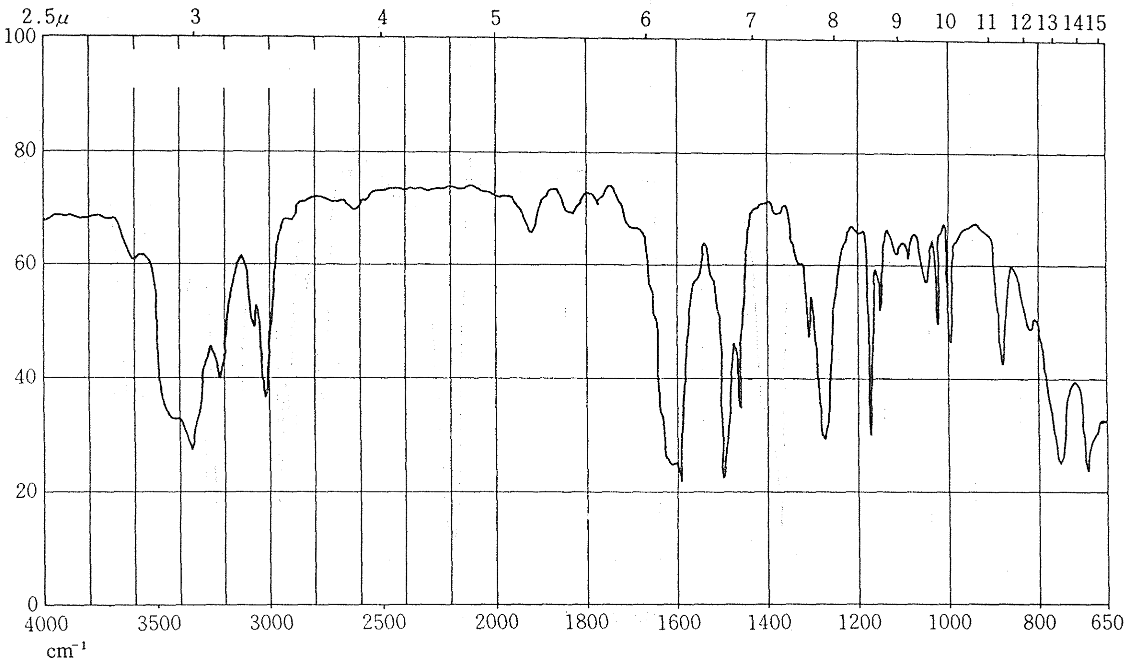


Fig. 6 Aniline

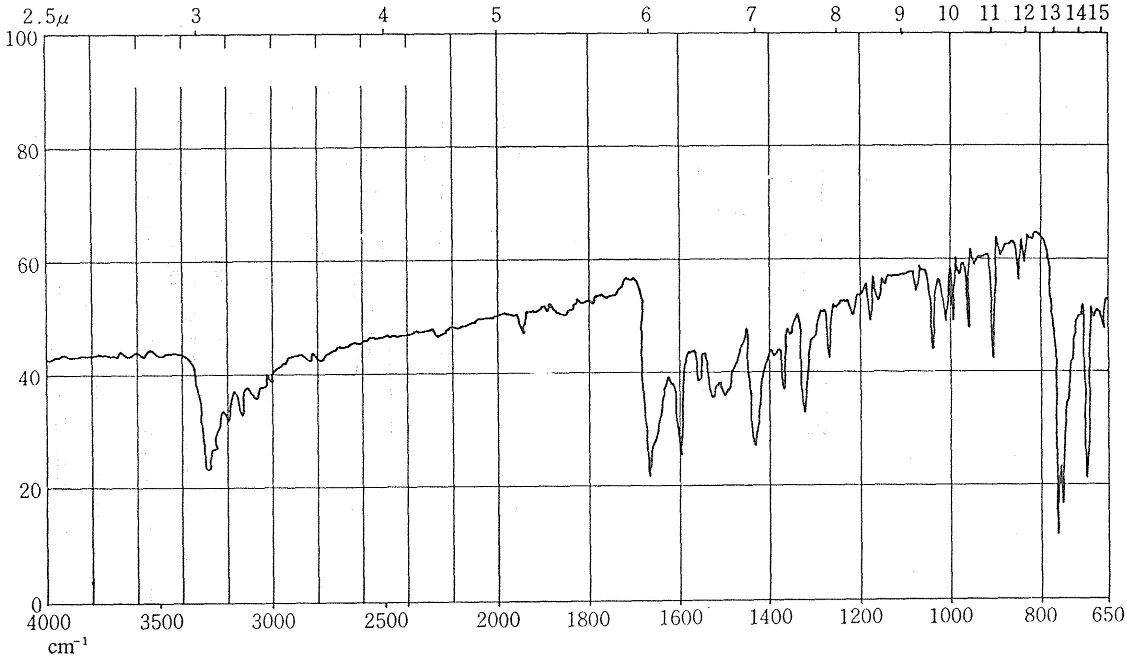


Fig. 7 Acetanilide

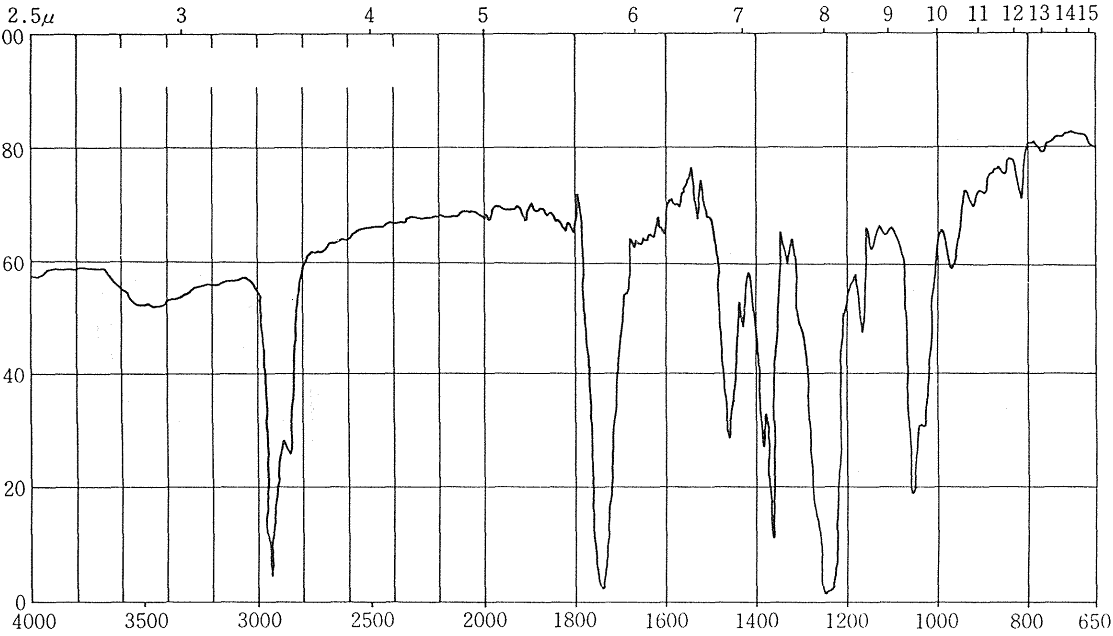


Fig. 8 Isoamilacetate

2-b. Decomposition of Polystylene

Polystylene, dissolved in benzene, is decomposed with heating the solution to be stylene-monomer. IR-spectrum of stylenemonomer is measured. Stylenemonomer is polymerized to be polystylene and its spectrum is measured also.

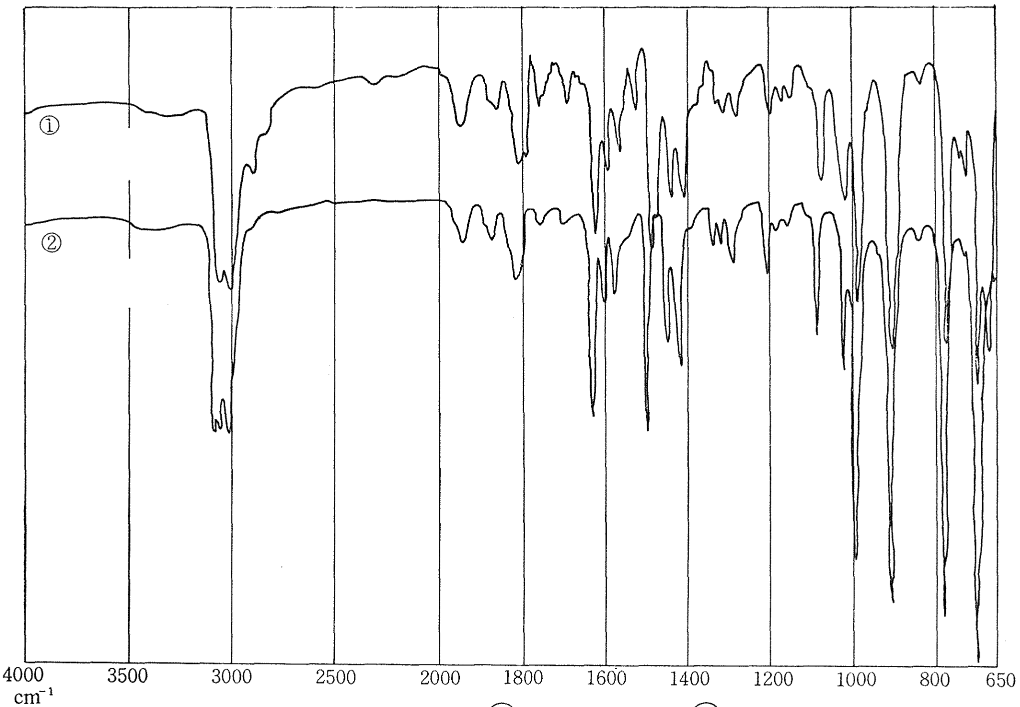


Fig. 9 Stylenemonomer ① by students ② standard

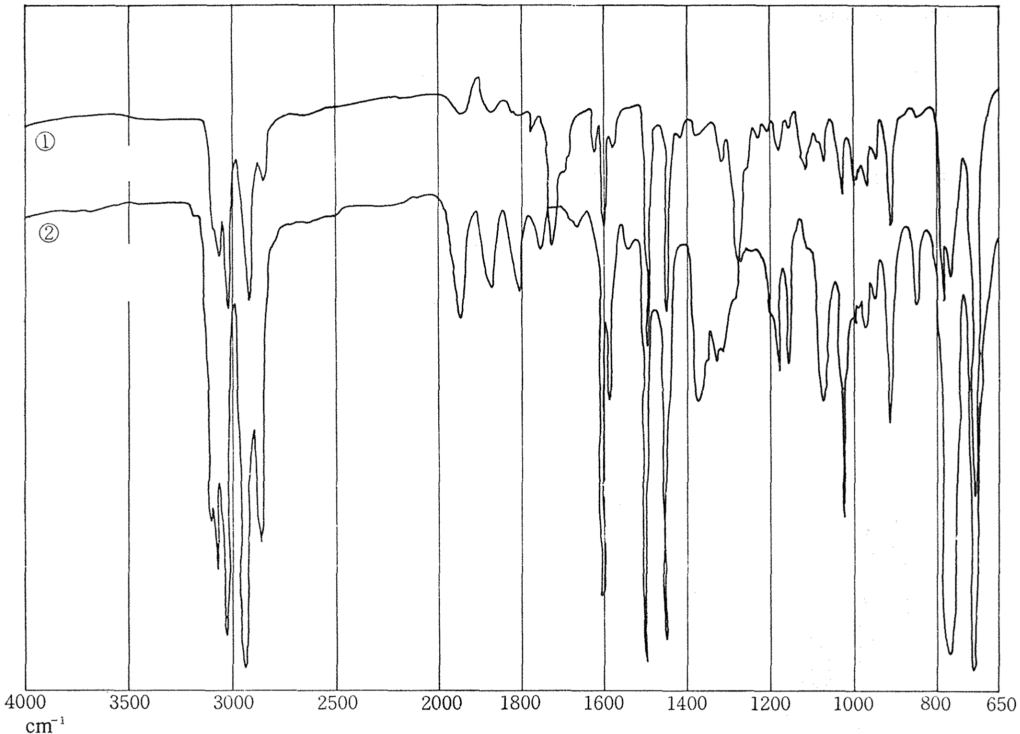


Fig. 10. Polystylene
① by students ② polystylene film

3. Microcomputers

3-a. Counting up Isomers of Alcohols and Alkanes

The number of isomers of saturated monohydric alcohols $C_nH_{2n+1}OH$ and alkanes C_nH_{2n+2} can be shown with an asymptitic formula.

If a series of the number of the isomers of the alcohols $C_nH_{2n+1}OH$ is chosen as a_n, the generating function of a_n is shown as next.

$$A(x)=a_0+a_1x+a_2x^2+\cdots\cdots+a_nx^n+\cdots\cdots \tag{7}$$

And the next function can be taken.

$$A(x)=1+\frac{x}{6}[\{A(x)\}^3+3A(x)A(x^2)+2A(x^3)] \tag{8}$$

The number of isomers of the alkane C_nH_{2n+2} can be taken with using A(x).

$$C(x)=P(x)-Q(x)+A(x^2) \tag{9}$$

Provided that

$$P(x)={}^{x}/_{24}[\{A(x)\}^4+6\{A(x)\}^2A(x^2)+3\{A(x)\}^2 8A(x)A(x)+6A(x^4)] \quad \ldots \quad (10)$$

$$Q(x)={}^{1}/_{2}[\{A(x)\}^2-2A(x)+A(x^2)] \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (11)$$

The beginning of the function C(x) is next.

$$C(x)=1+x+x^2+x^3+2x^4+3x^5+5x^6+9x^7+\cdots\cdots \quad \ldots\ldots\ldots\ldots\ldots \quad (12)$$

The computer programs of formula (8) (9) and the results are shown Fig. 11 and Fig. 12.

```
10 TIME$="00:00:00"
100 REM Enumeration of Isomer Number
110 REM by A.Kato
120 REM
130 DEFDBL A,P,Q,C
140 DIM A(30),A2(30)
150 DEFINT I,J,N
160 LPRINT "    N                    A                  C          TIME"
170 LPRINT
180 A(0)=1:A2(0)=1
190 FOP N=1 TO 30
200  N1=N-1
210  FOR I=0 TO N1                                      }
220   A(N)=A(N)+A(I)*A2(N1-I)                           }{A(x)}³
230  NEXT I                                             }
240  FOR I=0 TO N1 STEP 2                               }
250   A(N)=A(N)+3*A(I¥2)*A(N1-I                         }3A(x)A(x²)
260  NEXT I                                             }
270  A(N)=A(N)-(N1 MOD3 =0)*2*A(N1¥3)                    2A(x³)
280  A(N)=INT(A(N)/6+.5)                                 3{A(x²)}²
290  P=-(N1 MOD2 =0)*3*A2(N1¥2)
300  FOR I=0 TO N1                                      }
310   P=P+A2(I)*A2(N1-I)                                }{A(x)}⁴
320  NEXT I                                             }
330  FOR I=0 TO N1 STEP 2                               }
340   P=P+6*A(I¥2)*A2(N1-I)                             }6{A(x)}²A(x²)
350  NEXT I                                             }
360  FOR I=0 TO N1 STEP 3                               }
370   P=P+8*A(I¥3)*A(N1-I)                              }8A(x)A(x³)
380  NEXT I                                             }
390  P=P-(N1 MOD4 =0)*6*A(N1¥4)
400  P=INT(P/24+.5)                                      6A(x⁴)
410  FOR I=0 TO N                                       }
420   A2(N)=A2(N)+A(I)*A(N-I)                           }{A(x)}²
430  NEXT I                                             }
440  Q=A2(N)-2*A(N)-(N MOD2 =0)*A(N¥2)                  }
450  Q=INT(Q/2+.5)                                      }→Q(x)の計算
460  C=P-Q-(N MOD2 =0)*A(N¥2)                           }
470  LPRINT USING"#####";N;                                C(x)=P(x)-Q(x)+A(x²)
480  LPPINT USING"##################.";A(N);C;
485  LPPINT "          "+PIGHT$(TIME$.4)
490 NEXT N
500 END
```

Fig. 11 Computer program

```
 N                    A                 C          TIME

 1                    1                 1          0:03
 2                    1                 1          0:05
 3                    2                 1          0:09
 4                    4                 2          0:12
 5                    8                 3          0:15
 6                   17                 5          0:18
 7                   39                 9          0:21
 8                   89                18          0:25
 9                  211                35          0:28
10                  507                75          0:31
11                1,238               159          0:35
12                3,057               355          0:38
13                7,639               802          0:42
14               19,241             1,858          0:46
15               48,865             4,347          0:50
16              124,906            10,359          0:53
17              321,198            24,894          0:57
18              830,219            60,523          1:01
19            2,156,010           148,284          1:05
20            5,622,109           366,319          1:09
21           14,715,813           910,726          1:14
22           38,649,152         2,278,658          1:18
23          101,821,927         5,731,580          1:22
24          269,010,485        14,490,245          1:27
25          712,566,567        36,797,588          1:31
26        1,891,993,344        93,839,412          1:36
27        5,034,704,828       240,215,803          1:40
28       13,425,117,806       617,105,614          1:45
29       35,866,550,869     1,590,507,121          1:50
30       95,991,365,288     4,111,846,763          1:54
```

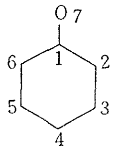
Fig. 12 Number of isomers A: alcohols C: alkanes

3-b. Orientation of the Aromatic Ring

The orientation of the aromatic ring is calculated with M.O method using the microcomputer. Fig. 13 Fig. 14.

```
<<<< MOLECULAR DIAGRAM >>>>

1.029  0.647  -----  -----  -----  0.647  0.238
0.647  1.010  0.670  -----  -----  -----  -----
-----  0.670  1.000  0.664  -----  -----  -----
-----  -----  0.664  1.010  0.664  -----  -----
-----  -----  -----  0.664  0.999  0.670  -----
0.647  -----  -----  -----  0.670  1.011  -----
0.238  -----  -----  -----  -----  -----  1.941
```



```
          FRONTIER                POLARIZABILITY   SUPER-                 LOCALIZATION
          ELECTRON DENSITY                         DELOCALIZABILITY       ENERGY

ortho-       0.209                    0.407             0.884                2.454
meta-        0.108                    0.397             0.832                2.539
para-        0.558                    0.402             0.879                2.474
```

Fig. 13 Phenol (ortho, para)

```
<<<< MOLECULAR DIAGRAM >>>>

 1.030   0.602   -----   -----   -----   0.603   0.404   -----   -----
 0.602   0.943   0.682   -----   -----   -----   -----   -----   -----
 -----   0.682   1.001   0.656   -----   -----   -----   -----   -----
 -----   -----   0.656   0.948   0.656   -----   -----   -----   -----
 -----   -----   -----   0.656   1.001   0.682   -----   -----   -----
 0.603   -----   -----   -----   0.682   0.943   -----   -----   -----
 0.404   -----   -----   -----   -----   -----   1.013   0.637   0.637
 -----   -----   -----   -----   -----   -----   0.637   1.561   -----
 -----   -----   -----   -----   -----   -----   0.637   -----   1.561

            FRONTIER                 POLARIZABILITY  SUPER-                 LOCALIZATION
            ELECTRON DENSITY                         DELOCALIZABILITY       ENERGY

ortho-         0.500                     0.432           0.779                 2.552
meta-          0.500                     0.395           0.828                 2.548
para-          0.000                     0.416           0.753                 2.625
```

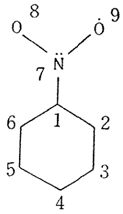


Fig. 14 Nitrobenzene (meta)

4. pH-meters

Let x be as next in the acid-base titration.

$$x \equiv \frac{\text{the added volume of base (acid)}}{\text{the initial volume of acid (base)}}$$

And if the acid or the base in the initial solution is defined to be p or q, and the base or the acid in the addition solution is defined to be r or s, so each initial concentration of acid and base will be shown as Cap, Cbq, Cbr, Cas.

More

$$A(m) \equiv \frac{\sum_{i=1}^{m}(i[H^+]^{m-i} \prod_{1\leqq j\leqq i} K_{aj})}{\sum_{i=0}^{m}([H^+]^{m-i} \prod_{1\leqq j\leqq i} K_{aj})} \quad \cdots\cdots\cdots\cdots\cdots\cdots \quad (13)$$

$$B(m) \equiv \frac{\sum_{i=1}^{m}\left(i\left(\frac{K_W}{[H^+]}\right)^{m-i} \prod_{1\leqq j\leqq i} Kb_j\right)}{\sum_{i=0}^{m}\left(\left(\frac{K_W}{[H^+]}\right)^{m-i} \prod_{1\leqq j\leqq i} Kb_j\right)} \quad \cdots\cdots\cdots\cdots\cdots\cdots \quad (14)$$

are defined, and Ap(As) shows the value of A(m) about the acid p(S), and Bq(Br) shows the value of B(m) about the base q(r), so the x is shown with the next formula

$$x = \frac{[\sum_{p}(A_pCa_p) - \sum_{q}(B_qCb_q)][H^+] + K_W - [H^+]^2}{[\sum_{r}(B_rCb_r) - \sum_{s}(A_sCa_s)][H^+] - K_W + [H^+]^2}$$

The x is calculated, and the titration curve is formulated and compared with the experimental data of pH meters on the system of the oxalicacid-NaOH and the system of the oxalicacid- (ammonia water, pyrydine solution).

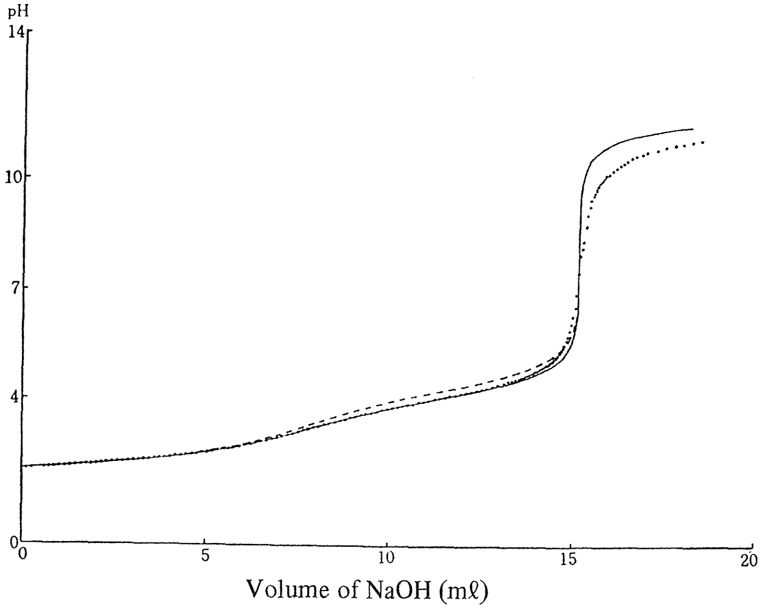


Fig. 15 Oxalic acid- NaOH

$Ca = 1.0238 \times 10^{-2}$ mol/l, $Cb = 4.05 \times 10^{-2}$ mol/l Oxalic acid $Ka_1 = 5.36 \times 10^{-2}$, $Ka_2 = 5.73 \times 10^{-5}$ (18°C) $Kw = 0.579 \times 10^{-14}$ (18°C)

---- (a) $\gamma = 1$ —— (b) Debye-Hückel …… (c) experiment

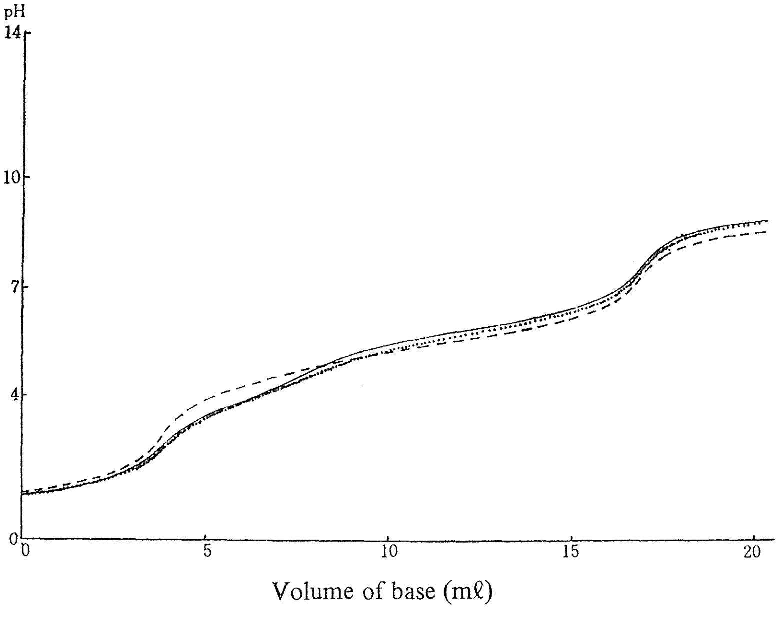


Fig. 16 Oxalic acid- NH_3, pyrydine

$Ca = 0.996 \times 10^{-1}$ mol/l, $Cb_1 = 0.335$ mol/l (NH_3), $Cb_2 = 0.432$ mol/l (C_5H_5N)
Oxalic acid $Ka_1 = 5.36 \times 10^{-2}$, $Ka_2 = 5.49 \times 10^{-5}$ (22.5°C) NH_3 $Kb_1 = 1.75 \times 10^{-5}$ (22.5°C), C_5H_5N $Kb_2 = 1.38 \times 10^{-9}$ $Kw = 0.832 \times 10^{-14}$ (22.5°C)