NOTAS DE MATEMATICAS
Nº 117

ON THE SEARCH FOR THE BEST CORRELATION BETWEEN GRAPH THEORETICAL INVARIANTS AND PHISICOCHEMICAL PROPERTIES

BY

DANIEL A. MORALES

AND

OSWALDO APAUJO

UNIVERSIDAD DE LOS ANDES
FACULTAD DE CIENCIAS
DEPARTAMENTO DE MATEMATICAS
MERIDA - VENEZUELA

1991

ON THE SEARCH FOR THE BEST CORRELATION BETWEEN GRAPH THEORETICAL INVARIANTS AND PHISICOCHEMICAL PROPERTIES.

BY

DANIEL A. MORALES AND OSWALDO ARAUJO

ON THE SEARCH FOR THE BEST CORRELATION BETWEEN GRAPH THEORETICAL INVARIANTS AND PHYSICOCHEMICAL PROPERTIES

Daniel A. Morales
Grupo de Química Teórica
Departamento de Química
Facultad de Ciencias
Universidad de los Andes
Mérida 5101, Venezuela

and

Oswaldo Araujo
Departamento de Matemática
Facultad de Ciencias
Universidad de los Andes
Mérida 5101, Venezuela

ABSTRACT

We have examined the correlation of Randić's connectivity index with the Hosoya topological index, Wiener number and the molecular identification number in the search for the most optimal functional relation between those indices and the boiling points of alkanes. We found that some functional relations used empirically in the literature can be understood using the known fact that the Randić index is the most successful single descriptor of molecular structure.

1. INTRODUCTION

It is well known that molecular topology determines a large number of molecular properties including not only those depending on the molecular size and shape such as boiling points, molecular volumes, solubilities, refractive indices, etc. but also the quantum mechanical characteristics of molecules such as energy levels, electronic populations etc. which depend, essentially, on the connectivity of the atoms [1].

Thus, it is of great interest for chemistry to have some quantitative measure reflecting the essential features of a given topological structure. Such measures are usually called topological indices or, more exactly, graph theoretical invariants, since these numbers are the same for isomorphic graphs [2]. These indices reflect in some way not only the size and shape of a molecule but also their connectivity, i.e. the way their atoms are linked.

Many topological indices have been developed through the years and correlated with many physicochemical properties [2-5]. Recently, Randić et al. [6] have made a critical study of the correlation of four indices: Wiener number (W), Hosoya's topological index (Z), Randić's connectivity index (χ), and the molecular identification number (ID) with the boiling points of alkanes. They found different functional forms for the correlations which lead to significant improvements in the

correlation coefficients compared to those using only the plain topological indices. However, the search for the best functional form was somewhat empirical. On the other hand, their study shows that there exists correlations among the different topological indices, although no mathematical relations where established. It is the purpose of this note to establish and test approximate functional relations among the four indices previously indicated and to explain, based on these relationships, why the functional forms proposed by Randić et al. work taking as a basis the good correlation between the boiling points of alkanes and Randic's connectivity index.

This paper is organized as follows. In section 2 we review the definitions of the four indices indicated above and proof their invariances. In section 3 we establish approximate relations between Randic connectivity index and Wiener number, Hosoya topological index, and the molecular identification index and test the expresions obtained with actual correlations. Also, in that section, we correlate the boiling points of the lower alkanes with the functional relations encountered. Section 4 is a summmary of our results.

2. Overview of Topological Indices.

We shall assume that the reader has some familiarity with the terminology of graph theory; Harary's book is a good reference [7]. Also, we suppose that all molecular species can be

represented by means of an appropriate chemical graph.

An invariant of a graph G is any number associated with G which has the same value for any graph isomorphic to G . In a connected graph G, the distance d(i,j) between two vertices i and j is the length of the shortest path joining them.

In what follows we review the Wiener index, Hosoya topological index, Randić connectivity index and the molecular identification number and prove their invariance.

Wiener Number

The Wiener number was introduced in 1947 by Wiener [8] and is based in the graph concept of distance. The Wiener number is identically equal to one-half the sum of the elements of the distance matrix of graph G [9], i.e.

$$W = \frac{1}{2} \sum_{ij} d_{ij} \qquad (1)$$

where the d_{ij}s are the coefficients of the distance matrix $D=(d_{ij})$.

The Wiener number of any graph G is an invariant. In fact, if G′ is a graph isomorphic to G, then f: G → G′ is a bijection which preserves adjacency. Now, if $D=(d_{ij})$ and $D'=(d'_{kl})$ are the distance matrices of G and G′, respectively, we have $d_{ij} = \min d(i,j) = d'_{f(i)f(j)}$, that is, W = W′, where W′ is the Wiener number of the graph G′.

For normal alkanes, i.e. unbranched alkanes, we have the

following formula

$$W_a = \frac{1}{6}\ (n^3 - n) \qquad (2)$$

where n is the number of vertices. The proof of the last expression is as follows: for an n-alkane the distance matrix can be written, in general, as,

$$D = \begin{bmatrix} 0 & 1 & 2 & \ldots & n-1 \\ 1 & 0 & 1 & \ldots & n-2 \\ 2 & 1 & 0 & \ldots & n-3 \\ \multicolumn{5}{c}{\ldots\ldots\ldots\ldots\ldots} \\ n-1 & n-2 & n-3 & . \; . & 0 \end{bmatrix} .$$

Since D is symmetric and the Wiener number is one-half the sum of the elements of the distance matrix, we can write W as the sum of each row over the diagonal of the matrix D. Thus,

$$W = \sum_{k=1}^{n-1} k + \sum_{k=1}^{n-2} k + \ldots. + 1 + 0$$

$$= \sum_{k=1}^{n-1} k(n-k)$$

$$= n \sum_{k=1}^{n-1} k - \sum_{k=1}^{n-1} k^2$$

$$= \frac{n(n-1)n}{2} - \frac{(n-1)n[2(n-1)+1]}{6}$$

$$= \frac{(n^3 - n)}{6} .$$

The Wiener number is an index which gives a measure of the branching of a graph [10]. Thus, the Wiener number of a branched molecule is less than that of a linear or less compact molecule. Platt [11] has suggested that the cubic root of the Wiener number is a measure of the mean distance among carbon atoms in a molecule and is, approximately, a measure of the probability that one part of a molecule be attracted by other part by van der Waals forces. Since its introduction, it has been found that this index correlates very well with properties such as boiling point, viscosity, surface tension and refraction index. On the other hand, it has been found that, in general, a system is at its minimum of energy when its Wiener's number is a minimum [12] . This last finding could be useful in the search for the most probable geometry of clusters.

The Randic Connectivity Index

The Randić index χ depends on the graph concept of degree [13] . It is defined by

$$\chi = \Sigma \ (1/mn)^{1/2}. \qquad (3)$$

This summation is over all edges in the graph G and it includes one term for each edge in G. The variables m and n are the degrees

of the adjacent points joined by each edge. Since the degree of any graph is an invariant, χ is also an invariant.

Let G be the graph of a normal alkane, then

$$\chi_{4+n'} = \sqrt{2} + (1+n')/2, \qquad (4)$$

where 4+n' is the number of vertices and n'=-1,0,1,2,...It is clear that if n'=-1 then $\chi_3 = \sqrt{2}$. Now assume n'> -1. By the induction hypothesis

$$\chi_{4+n'} + 1/2 = \sqrt{2} + (1+n')/2 + 1/2 = \sqrt{2} + (1+(n'+1))/2$$

$$= \chi_{4+(n'+1)}.$$

Therefore, the formula above is valid for any n'> -1.

It has been found that the Randić index is the one which presents the best correlation with the physicochemical properties of many substances. Randić's index is also known as the path-one connectivity index. This comes from the fact that χ is calculated summing over all paths of length one in the structural graph. By a natural extension it is possible to consider additional indices corresponding to paths of lengths greater than one [14] .

Hosoya Topological Index

The Hosoya index of a graph G is based on the count of

nonadjacent edges of G and is defined as [9]

$$Z = \sum_{k=0}^{m} p(G,k), \qquad (5)$$

where p(G,k) represents the number of different ways of selecting k nonadjacent edges in graph G, and the summation extends over all the m edges of the graph. By definition, p(G,0)=1 and p(G,1) is equal to the number of edges.

Since every isomorphism of a graph preserves both adjacency and nonadjacency, we conclude that the Hosoya index is an invariant of G.

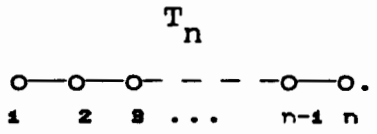
The Fibonacci numbers are integers F_n defined by

$$F_n = F_{n-1} + F_{n-2},\ n \geq 2\ ;\ F_0 = F_1 = 1.$$

They have a simple combinatorial meaning: F_{n+1} is the number of subsets of {1,...,n} such that no two elements are adjacent [15].

By definition, the Fibonacci number f(G) of a graph G with vertex set V and edge set E is the total number of subsets S of V such that any two vertices of S are not adjacent [16].

The sequence {1,...,n} can be regarded as the vertex set of the graph T_n:



Hence, for normal alkanes, the Hosoya index is given by

$$Z = f(T_n) = T_{n+1} = (1/\sqrt{5})\left[\left((1+\sqrt{5})/2\right)^{n+1} - \left((1-\sqrt{5})/2\right)^{n+1} \right]. \quad (6)$$

Molecular Identification Index

The molecular identification index [17] of a graph G is defined as the sum of weighted path numbers. Each path of length zero is given a weight of unity and for paths of length greater than zero the weight is equal to the product of $(1/mn)^{1/2}$ terms, one term for each edge included in the path, where m and n are the degrees of the vertices joined by the edge. In mathematical terms

$$ID = \sum_i \omega_{oi} + 1/2 \sum_{ij} \omega_{ij}, \quad (7)$$

where ω_{oi} is the path-weight for all paths of lenghts zero, and ω_{ij} is the path-weight corresponding to all paths of length greater than zero.

Since the Randić index and the number of vertices of G are invariants then the molecular identification index is also an

invariant.

It is easy to see that, for normal alkanes,

$$ID = n + \sqrt{2} \sum_{i=0}^{n-3} (1/2^i) + s \qquad (8)$$

where $n \geq 3$ is the number of vertices and

$$s = 1/2^{n-2} + \sum_{i=0}^{n-3} (i/2^{n-i-2}). \qquad (9)$$

Using the expression for the geometric progression the preceding equation can also be written as

$$ID = 2\ (2^{2-n} + 2^{1-n} + n-2\ ) + (2 - 2^{3-n})\sqrt{2}. \qquad (10)$$

3. Relations Between Indices

As has been pointed out previously, the Randic index is the most successful single descriptor of molecular properties; however, as it is obvious from Fig. 1, where we plot the correlation between the experimental boiling points of 21 alkanes, tabulated in Table I, and Randic´'s connectivity index, the linear correlation does not fit adequately the experimental data due to the curvature of the plot. In Fig.2 we show a fitting of the data to a second-degree polynomial in χ, demonstrating the best correlation found in the fitting procedure in this case.

From the preceding analysis, it is obvious that a search for the best correlation of physicochemical properties with topological indices is in order.

In this section we derive and test approximate expressions between the index of Randić and the Wiener number, Hosoya topological index , and the molecular identification index. The relations obtained are derived from exact formulas for linear alkanes, however **since the change in a topological index with the branching is small for small branching, we suppose that the functional relation obtained for linear alkanes is also valid for branched ones except that we allow the coefficients to vary.** We then make a correlation analysis based on the functional relations derived and the actual values for the topological indices of alkanes C_2 through C_7.

a. Relation between Randic's index and Wiener number.

From eqs. (2) and (4) above for normal alkanes we can derive the following approximate relation between χ and W:

$$\chi = A_R + B_R\ (6W)^{1/3} + C_R\ (6W)^{-1/3} + \ldots \qquad (11)$$

where $A_R = \sqrt{2}-3/2 \cong -0.09$, $B_R = 1/2$, $C_R = 1/6 \cong 0.17$, ...This equation was derived by approximately solving the resulting cubic equation in n in terms of W and then substituting the result in eq.(4). In Table I we reproduce the values of the four topological

indices considered here for the alkanes C_2-C_7. A linear regression analysis of the values of χ vs $(6W)^{1/2}$, no including ethane, leads to the following coefficients for the correlation : A_R = - 0.12, and B_R = 0.50 with a correlation coefficient (c.c) of 0.9906 and a standard deviation (s.d.) of 0.0817. If we include ethane then the results are A_R= -0.00394, B_R= 0.483 with a c.c of 0.9920 and a s.d. of 0.0878. This correlation is plotted in Fig.3. Thus, from this result we can conclude that since Randic's index presents a good correlation with the boiling points of the 21 alkanes listed in Table I (c.c of 0.9914 and a s.d. of 6.746) then a good correlation will be shown between the boiling points and the cubic root of the Wiener number; this is indeed what we find; the correlation obtained is given by

$$B.P. = -146.2 + 64.87\ W^{1/3}$$

with a c.c. of 0.9951 and a s.d. of 5.082 (data plotted in Fig. 4). This represents an improving over the correlation between the boiling points and the the first power of the Wiener number which gives a c.c. of 0.9432 and a s.d. of 17.09.

Randić et al.[6] have tested other powers of W in the correlation with the boiling points of the alkanes listed in Table I and found that a still better correlation will be obtained using $W^{1/4}$. In a correlation study of boiling points

and $W^{1/3}$ we found that a functional dependence of the form

$$BP = a + b\, W^{1/3} + c/W^{1/3} \qquad (12)$$

suggested by expression (11), with a= - 1.118×10^{2}, b= 5.774x10, and c= -3.503x10 gives a c.c. 0.9962 and a s.d. of 4.598 which are closed to those obtained from the correlation between boiling points and $W^{1/4}$ i.e. 0.9963 and 4.417 [6].

b. Relation between Randic's Index and Hosoya Topological Index.

In order to derive a relation between the Randic index and the Hosoya index we will approximate the expression (6). This is obtained by simple neglecting the term $[(1-\sqrt{5})/2]^{n+1}$ in (6), obtaining

$$Z \simeq (1/\sqrt{5})[(1+\sqrt{5})/2]^{n+1} \qquad (6')$$

Starting from eqs. (4) and (6') above we have derived the following approximate expression which relates χ and Z for linear alkanes

$$\chi = A_H + B_H \ln Z \qquad (13)$$

where

$$A_H = \sqrt{2} - 2 - \ln 5/ (4 \ln \alpha) \cong 0.250$$

$$B_H = 1/ 2 \ln \alpha \cong 1.039$$

and α is the Golden Number $(1+\sqrt{5})/2$.

Using the values for χ and Z from Table I a correlation analysis of χ vs ln Z, no including ethane, produces the following results: A_H= 0.300, B_H = 1.024 with a c.c. of 0.9988 and a s.d. of 0.0286. If we include the data for ethane we obtain A_H=0.2956, B_H=1.026 with a c.c. of 0.9992 and a s.d. of 0.0279 (see Fig.5). This correlation also explains previous correlations of boiling points of alkanes with the logarithm of Z. For the 21 alkanes listed in Table I we find

$$BP = -121.95 + 74.99 \ln Z$$

with a c.c. of 0.9902 and a s.d. of 7.185 (Fig.6), a large improving over the correlation of boiling points with Z (c.c.=0.9128, s.d. = 21.01).

Randic et al. [6] tested, empirically, several functional relations of powers of Z and found good correlations, specially for negative powers. This finding can be explained using the preceding discussion. Since Z^x can be written in a power series of

ln Z as

$$Z^x = \exp(x \ln Z) = 1 + x \ln Z + \frac{1}{2} x^2 \ln^2 Z + \ldots \qquad (14)$$

we see that Z^x is proportional to lnZ and that a correlation of Z^x with boiling points, for small x, will give good correlations coefficients. Randic et al. find the best fitting for x= -1/3 (using only fractional powers). The nonlinear terms in the expansion (14) above can be thought as coming from the nonlinear terms neglected in eq.(6) when the approximate formula (13) was obtained. The expansion (14) also suggests that a still better correlation can be obtained between boiling points and Hosoya's topological index by the following functional expression

$$BP = a_H + b_H \ln Z + c_H \ln^2 Z \qquad (15)$$

which, in turn, can be thought as coming from a nonlinear relationship between Randic´'s index and Hosoya's topological index, of the form

$$\chi = A' + B' \ln Z + C' \ln^2 Z \qquad (16)$$

Indeed, a fitting of Randic´'s index and Hosoya's index to the functional relation (16) produces the following result

$$\chi = 0.2755 + 1.049 \ln Z - 5.83\times10^{-3} \ln^2 Z$$

with a c.c. of 0.9992 and a s.d. of 0.0286.

A fitting of the data given in Table I to the functional relation given by eq.(15) gives the following coefficients: a_H=-169.92, b_H=130.32 and c_H=-13.93, with a c.c. of 0.9976 and a s.d. of 3.657 (Fig.7). These results are very closed to those obtained using $Z^{-1/3}$ (c.c = 0.9976, s.d. = 3.547).

Also, since $A_H < B_H$ lnZ in eq.(13) we can rewrite that equation as

$$\chi = B_H \ln Z \, [\, 1 + A_H/B_H \ln Z] \cong B_H \ln Z. \qquad (17)$$

Randic´ found that the best correlation is obtained using $\chi^{1/3}$; then we can write eq.(17) as

$$\chi^{1/3} = B_H^{1/3} (\ln Z)^{1/3}. \qquad (18)$$

Thus, a correlation of boiling points and $(\ln Z)^{1/3}$ must also give a better fitting than the correlation using lnZ. In fact, a regression analysis shows that, for the 21 alkanes listed in Table I,

$$BP = -387.56 + 335.56 (\ln Z)^{1/3}$$

with a c.c. of 0.9976 and a s.d. of 3.548 which are closed to those obtained using $Z^{-1/2}$ (Fig.8).

c. Relation between Randic's Connectivity Index and the Molecular Identification Index.

If we combine eqs.(4) and (10) we find a relation between Randic's topological index and the index of molecular identification given by

$$ID = a_{ID} \exp(-b_{ID} \chi) + c_{ID} \chi + d_{ID} \qquad (19)$$

where

$$a_{ID} = 2^{2\sqrt{2}}\left(\frac{3}{2} - \sqrt{2}\right),\ b_{ID} = \ln 4\ ,\ c_{ID} = 4,\ d_{ID} = 2(1-\sqrt{2}) \cong -0.8284$$

Since the first term in eq.(19) decays very rapidly with χ we can see that the relation between ID and χ is approximately linear. A linear regression analysis, using the data in Table I, and no including ethane, produces the following values: c_{ID}= 4.004 and d_{ID}= -0.3149 with a c.c. of 0.9828 and a s.d. of 0.450. If we include ethane then we get c_{ID} = 4.13 and d_{ID} = -0.667, with a correlation coefficient of 0.9876 and a s.d. of 0.457 (Fig.9). Using ID directly in a correlation analysis with boiling points

gives

$$B.P.= -129.685 + 17.514\ ID$$

with a c.c. of 0.9920 and a s.d. of 6.496 (Fig.10). A slight improving on the correlation is found using the fact that $\chi^{1/3}$ gives the best index. In this way from eq.(19) above we find that $ID^{1/3}$ is proportional to $\chi^{1/3}$. Thus, a regression analysis of boiling points and $ID^{1/3}$ gives

$$BP = -396.471 + 207.641\ ID^{1/3}$$

with a c.c. of 0.9922 and a s.d. of 6.406 (Fig.11). Randić et al. find that the best correlation is obtained using $ID^{1/2}$. The deviation in the powers 1/3 and 1/2 is, presumably, due to the neglect of the exponential term in eq.(19).

4. Conclusions

In this paper we have done an analysis of the existing correlations which exist among four important topological indices: Randić connectivity index, Wiener number, Hosoya topological index and the molecular identification index. We have established approximate relations which have been tested. The functional relations have then been used in establishing correlations with the boiling points of alkanes. Since it has been found that the

Randić index and its one-third power gives the best correlation with boiling points [6], we have used the functional relations among the Randić index and the three other indices mentioned above to find the best functional form for the correlation between those indices and the boiling points of alkanes, explaining, in this way, some empirical findings of Randić et al. [6].

The analysis of this paper also corroborates a fact point out by Randić: due the correlation among indices, it is going to be more difficult than anticipated to arrive at new invariants that have novel different structural bases and cannot be simply (if not trivially) related to those already existing [6].

REFERENCES

[1] D.H. Rouvray, Sci. Am. 255 (1986) 40.

[2] D.H. Rouvray, Am. Sci. 61 (1973) 729.

[3] N. Trinajstić, **Chemical Graph Theory** (CRC Press, Boca Raton, Florida, 1983). Vol. II.

[4] R.B. King and D.H. Rouvray, eds., **Graph Theory and Topology in Chemistry** (Elsevier, Amsterdam, 1987) section B.

[5] D.H. Rouvray, J. Comput. Chem. 8 (1987) 470.

[6] M. Randić, P.J. Hansen and P.C. Jurs, J. Chem. Inf. Comput. Sci. 28 (1988) 60.

[7] F. Harary, **Graph theory** (Addison-Wesley, Reading, Mass., 1972).

[8] H. Wiener, J. Am. Chem. Soc. 69 (1947) 17.

[9] H. Hosoya, Bull. Chem. Soc. Japan, 44 (1971) 2332.

[10] D.H. Rouvray, Discrete Appl. Math. 19 (1988) 317.

[11] J.R. Platt, J. Phys. Chem. 56 (1952) 328.

[12] D. Bonchev, O. Mekenyan and H.G. Fritsche, Phys. Stat. Sol. 55A (1979) 181; ib. 56A (1979) 607; Zeit. Phys. Chem. Leipzig, 265 (1984) 959; J. Cryst. Growth, 49 (1980) 90.

[13] M. Randić, J. Am. Chem. Soc. 97 (1975) 6609.

[14] L.B. Kier, W.J. Murray, M. Randić and L.H. Hall, J. Pharm. Sci. 65 (1976) 1226.

[15] L. Comtet, **Advanced Combinatorics** (D. Reidel, Dordrecht, Holland, 1974) p. 45.

[16] H. Prodinger and R.F. Tichy, Fibonacci Quarterly 20 (1982) 16.

[17] M. Randić, J. Chem. Inf. Comput. Sci. 24 (1984) 164.

Acknowledgement

We thank the CDCHT of the Universidad de los Andes for its support.

Table I. Experimental boiling points of lower alkanes and values of the Randic´ connectivity index χ, Wiener number W, Hosoya topological index Z, and the molecular identification index ID.

Compound	bp (obsd), °C	Randic´ index (χ)	Wiener no.(W)	Hosoya index(Z)	ID
ethane	-88.63	1.000	1	2	3.0000
propane	-42.07	1.414	4	3	4.9142
2-methylpropane	-11.73	1.732	9	4	6.7321
n-butane	-0.50	1.914	10	5	6.8713
2,2-dimethylpropane	9.50	2.000	16	5	8.5000
2-methylbutane	27.85	2.270	18	7	8.6968
n-pentane	36.07	2.414	20	8	8.8499
2,2-dimethylbutane	49.74	2.561	28	9	10.4660
2,3-dimethylbutane	57.99	2.643	29	10	10.5236
2-methylpentane	60.27	2.770	32	11	10.6792
3-methylpentane	63.28	2.808	31	12	10.6759
n-hexane	68.74	2.914	35	13	10.8391
2,2-dimethylpentane	79.20	3.061	46	14	12.4490
2,4-dimethylpentane	80.50	3.126	48	15	12.5092
2,2,3-trimethylbutane	80.88	2.943	42	13	12.2931
3,3-dimethylpentane	86.03	3.121	44	16	12.4427
2,3-dimethylpentane	89.78	3.181	46	17	12.5052
2-methylhexane	90.05	3.270	52	18	12.6704
3-methylhexane	91.85	3.308	50	19	12.6600
3-ethylpentane	93.48	3.346	48	20	12.6692
n-heptane	98.42	3.414	56	21	12.8338

FIGURE CAPTIONS

Figure 1. Correlation between the observed boiling points of the C_2-C_7 alkanes and the connectivity index χ. Linear regression analysis.

Figure 2. Correlation between the observed boiling points of the C_2-C_7 alkanes and the connectivity index χ. Parabolic regression analysis.

Figure 3. Correlation between the connectivity index χ and the third-power of the Wiener number.

Figure 4. Correlation between the boiling points of the C_2-C_7 alkanes and the third-power of the Wiener number.

Figure 5. Correlation between the connectivity index χ and the logarithm of the Hosoya index Z. Linear regression analysis.

Figure 6. Correlation between the boiling points of the C_2-C_7 alkanes and the logarithm of the Hosoya index Z. Linear regression analysis.

Figure 7. Correlation between the boiling points of the C_2-C_7 alkanes and the logarithm of the Hosoya index Z. Parabolic regression analysis.

Figure 8. Correlation between the boling points of the C_2-C_7 alkanes and the one-third power of the logarithm of the Hosoya index Z.

Figure 9. Correlation between the molecular identification number ID and the connectivity index χ.

Figure 10. Correlation between the boiling points of the C_2-C_7 alkanes and the molecular identification index ID.

Figure 11. Correlation between the boiling points of the C_2-C_7 alkanes and the one-third power of the molecular identification index ID.

Fig.1.

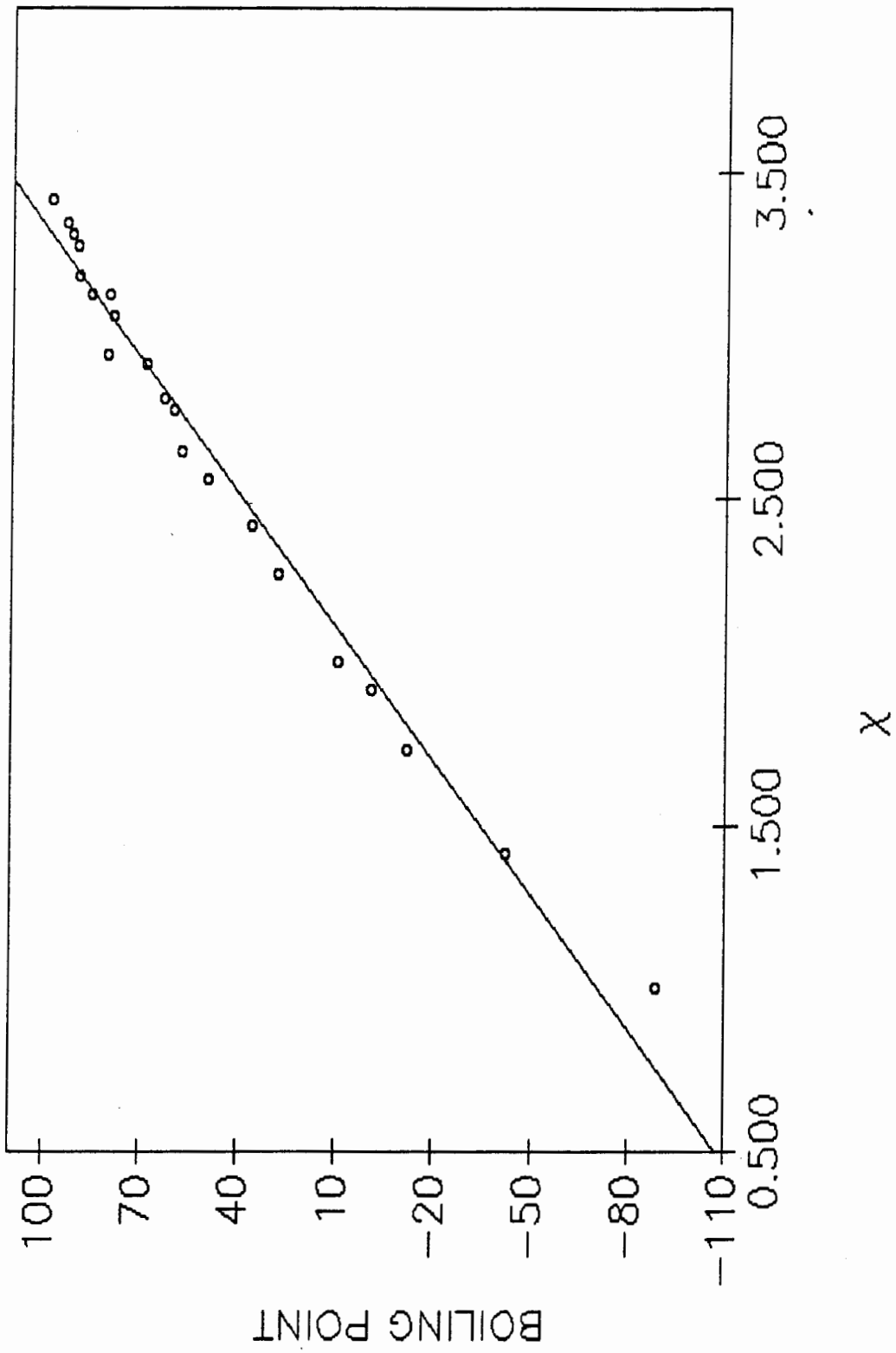


Fig.2.

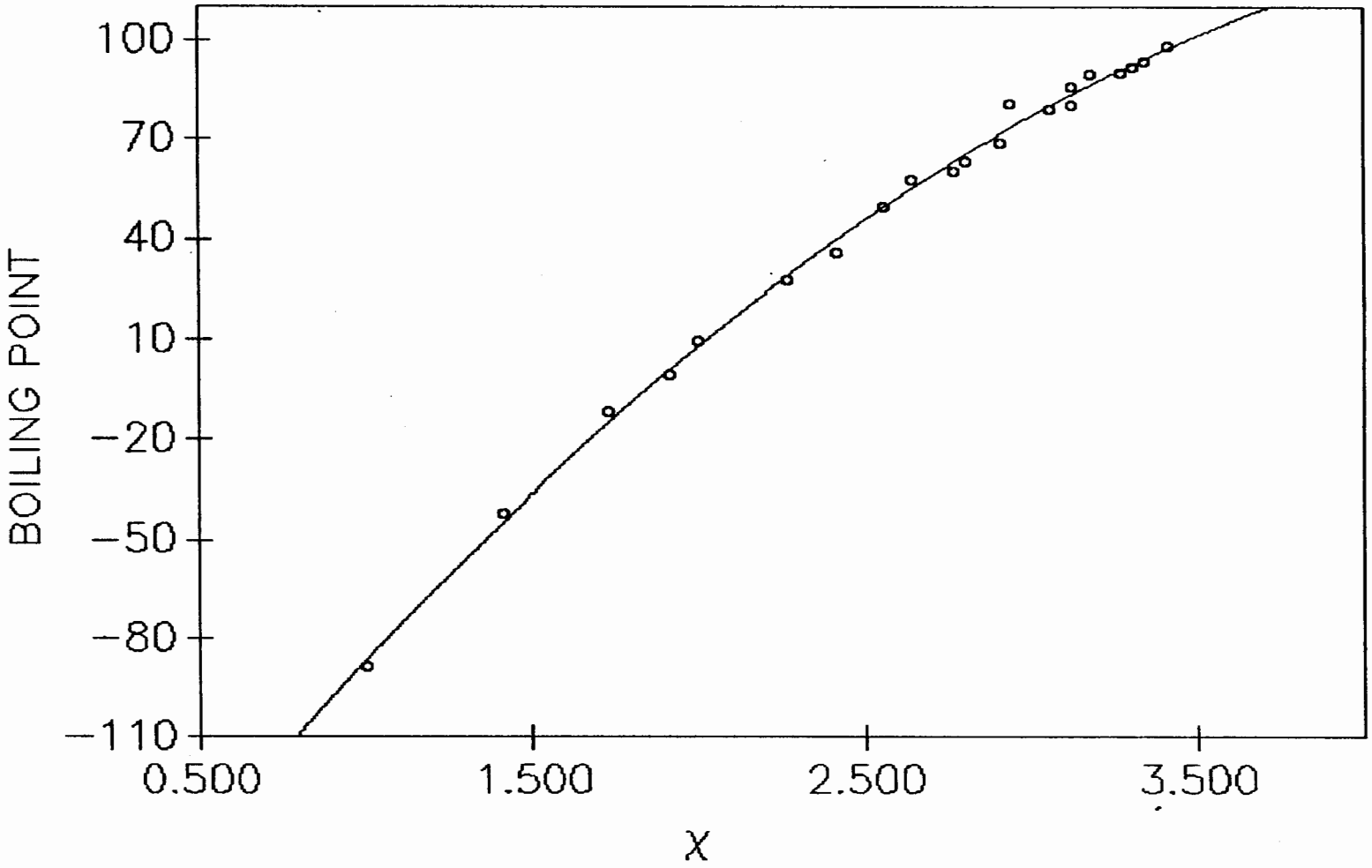


Fig.3.

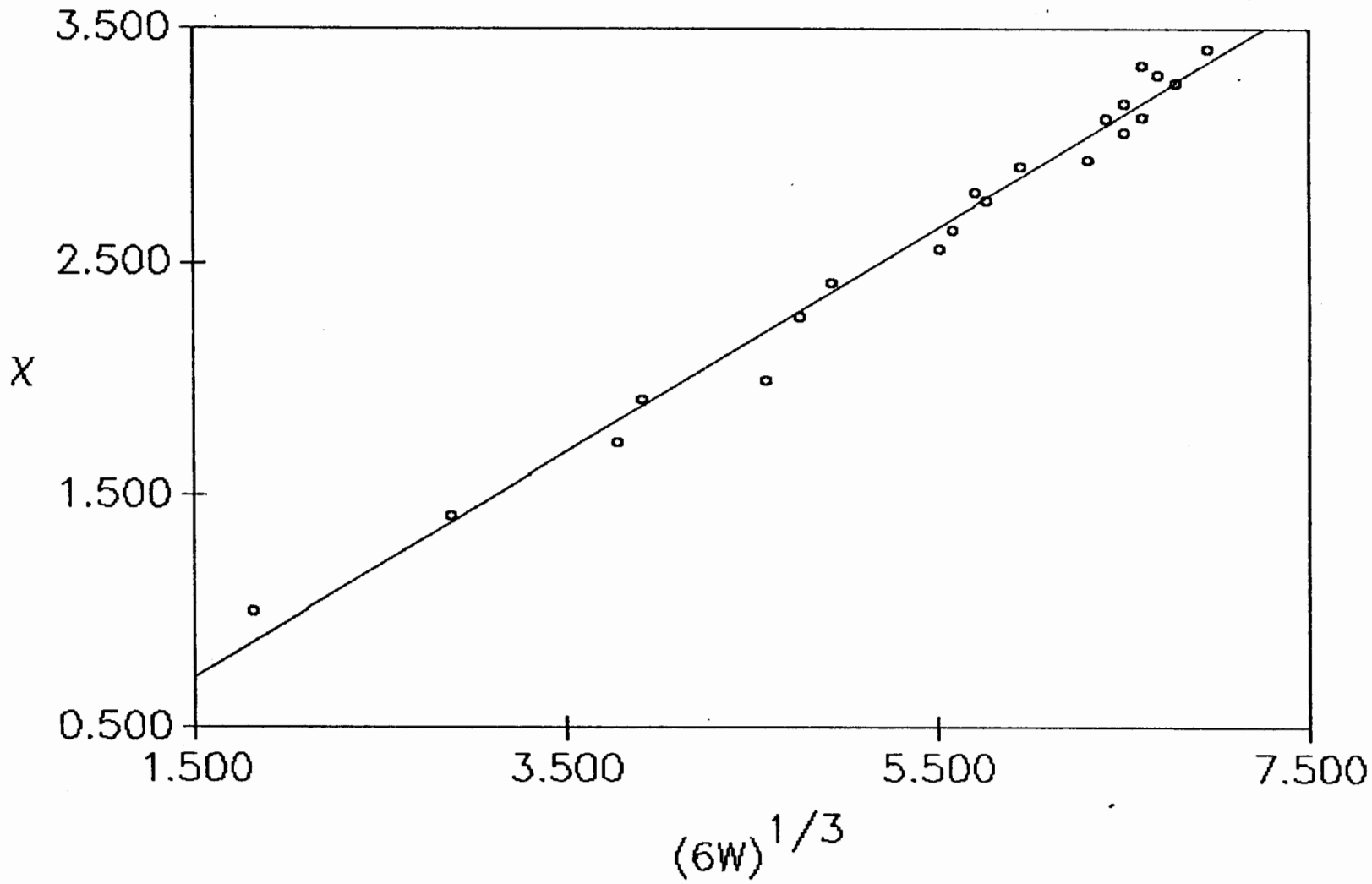


Fig.4.

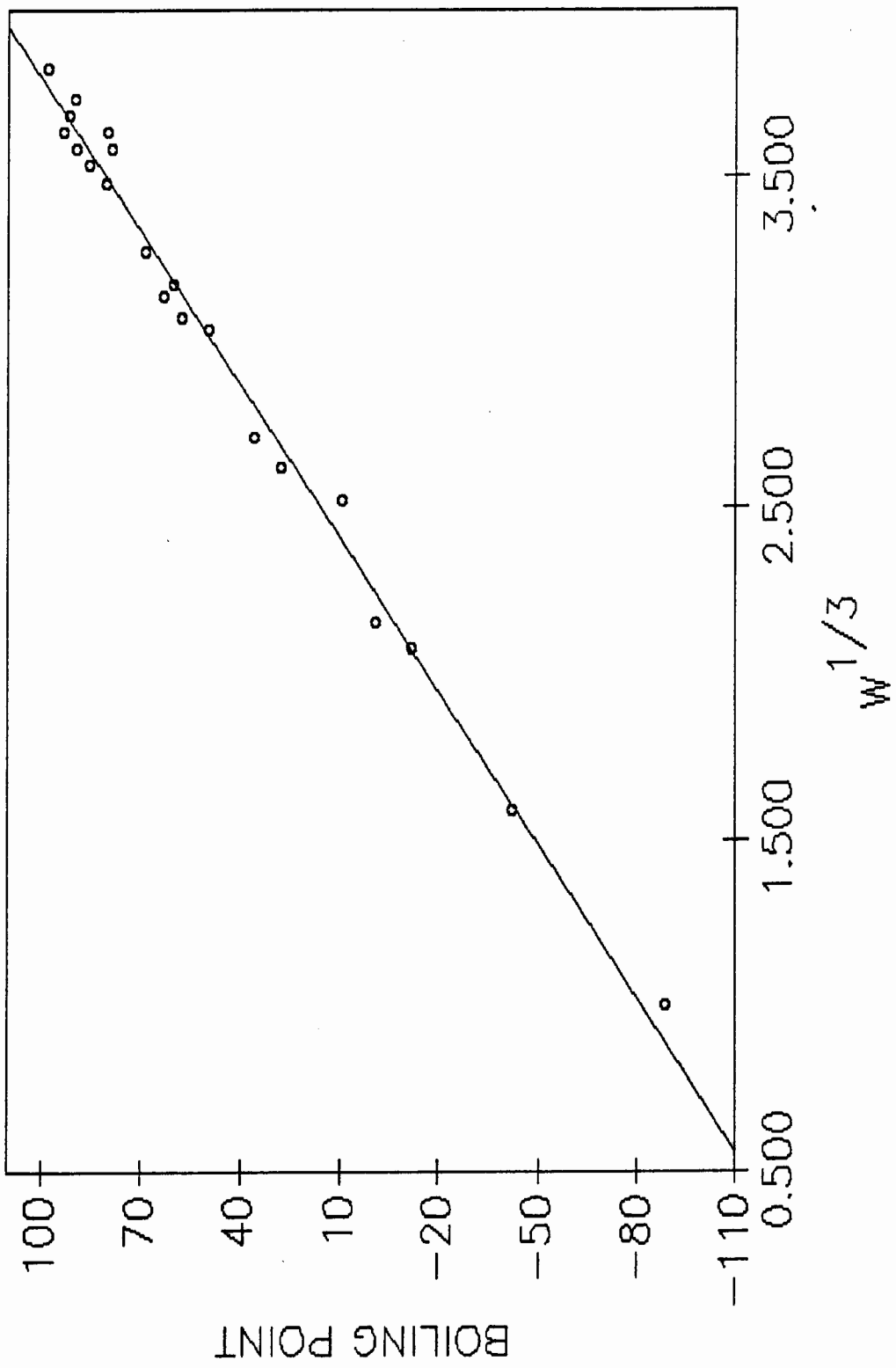


Fig.5.

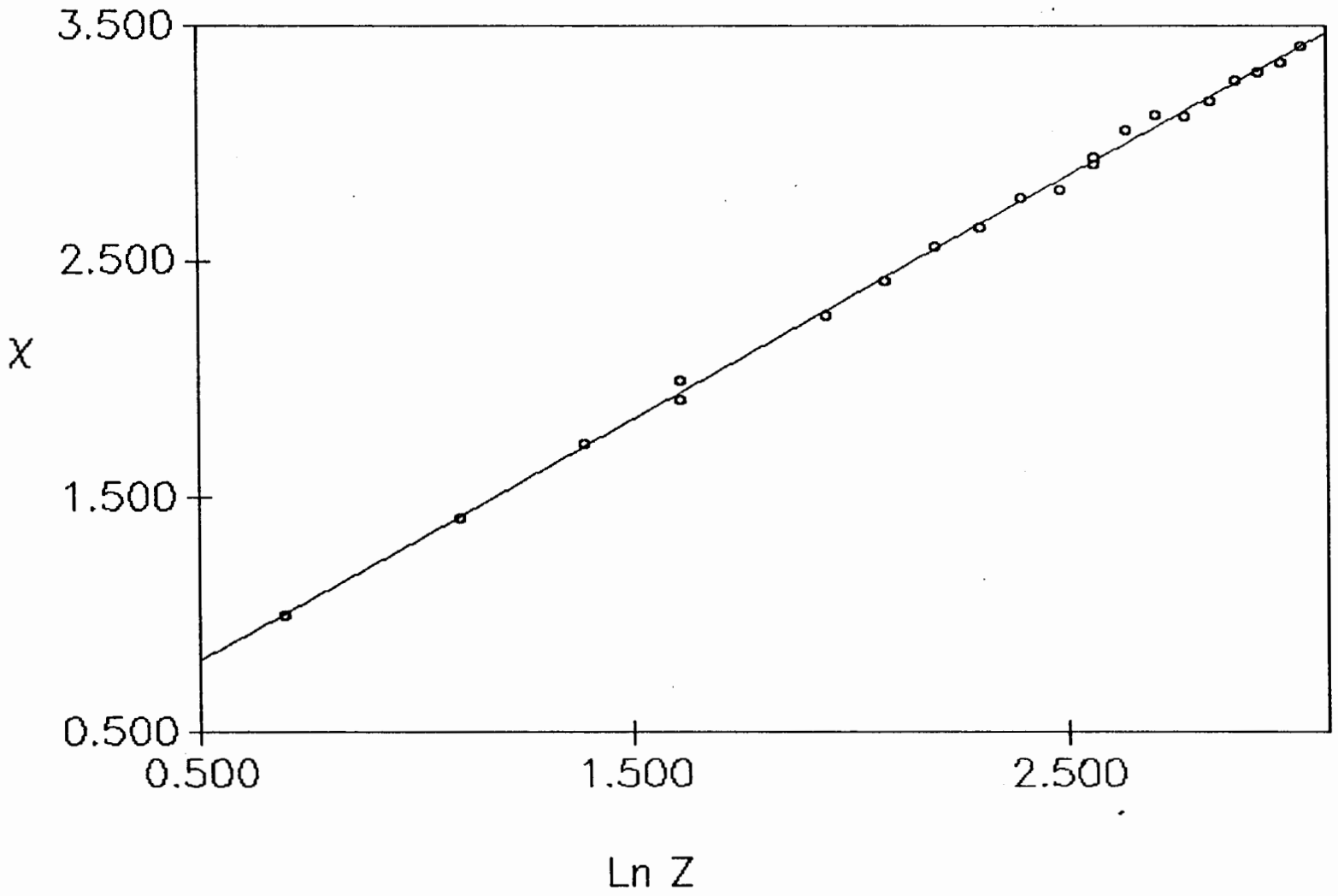


Fig.6.

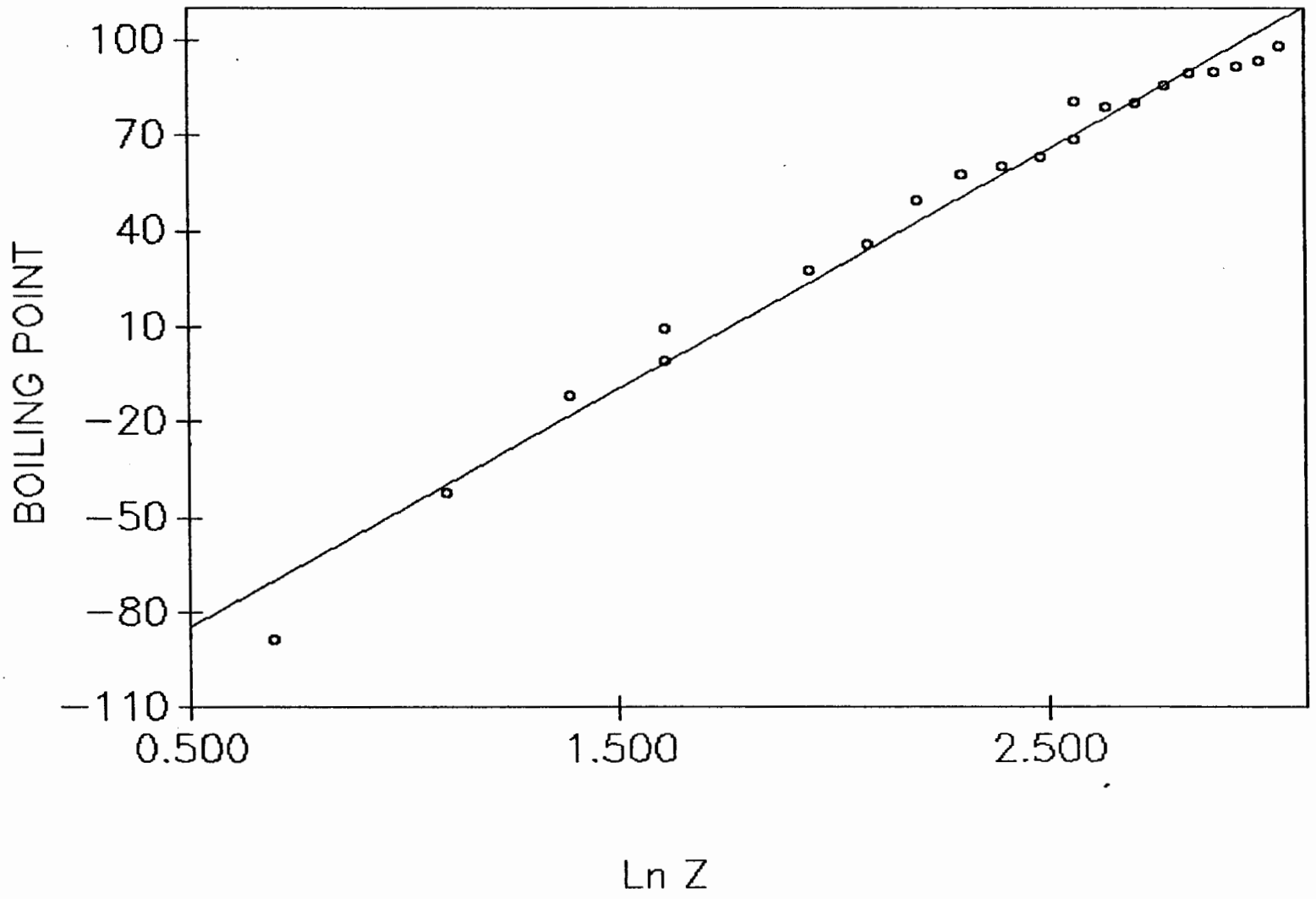


Fig.7.

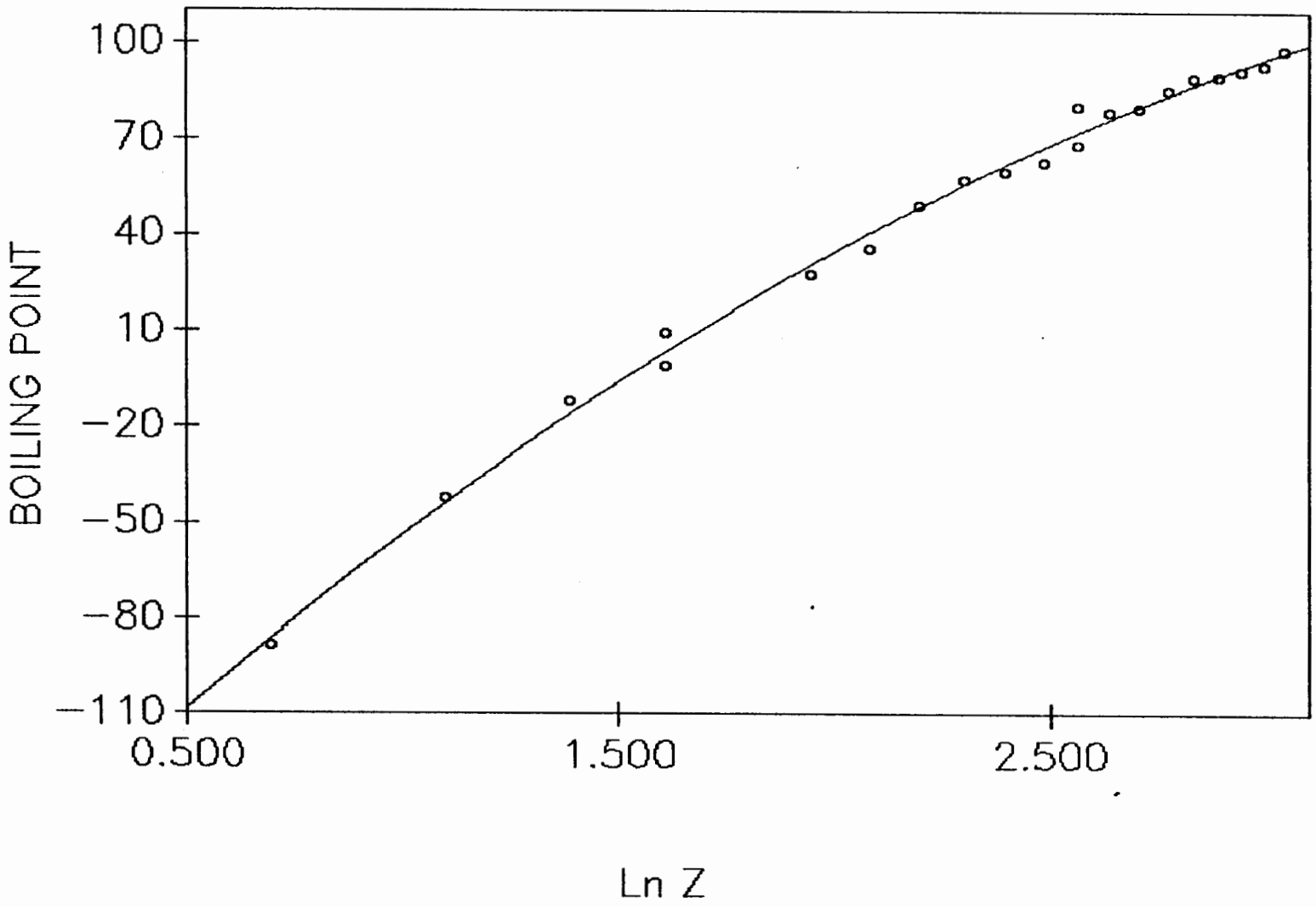


Fig.8.

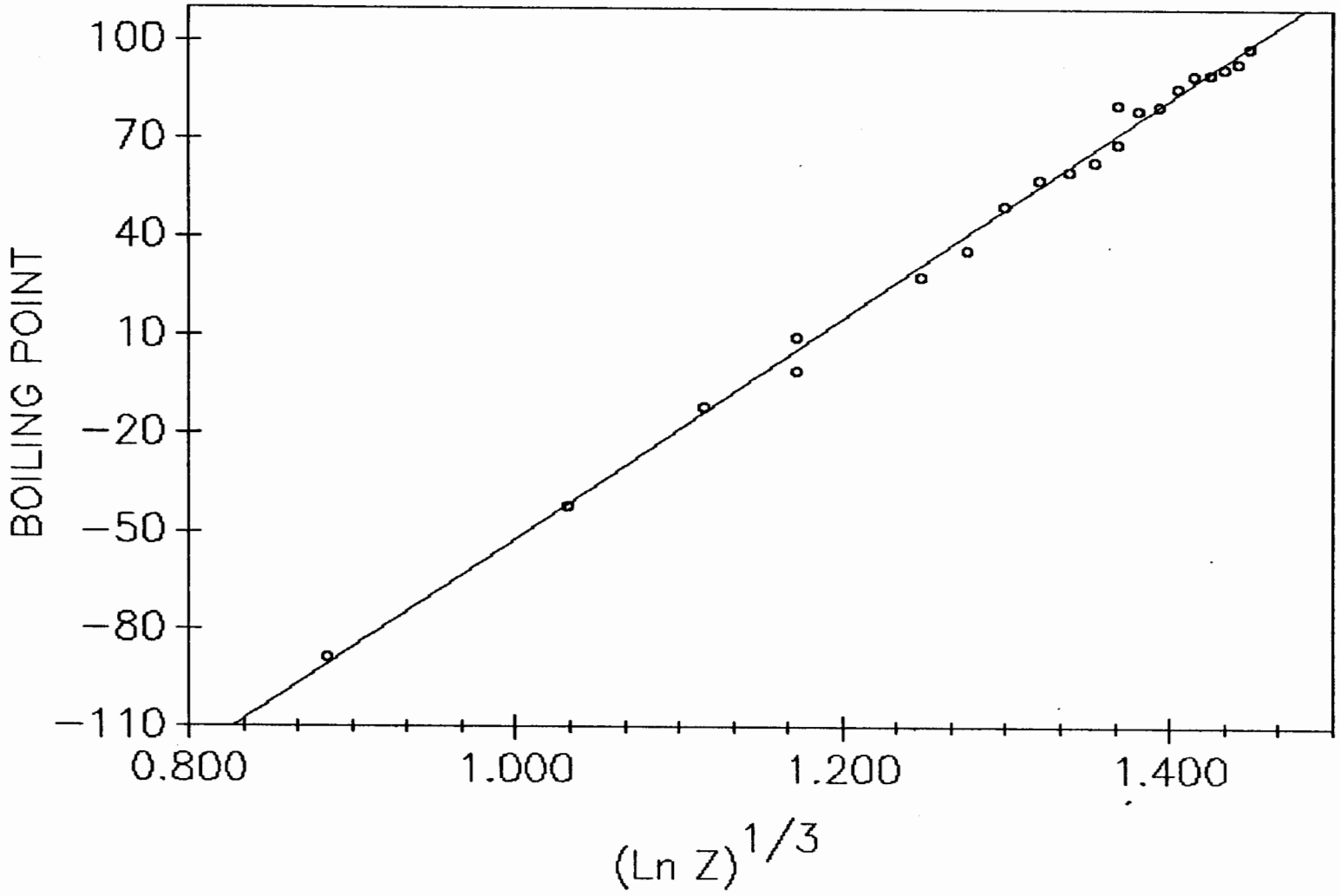

100
70
40
10
−20
−50
−80
−110
BOILING POINT
0.800
1.000
1.200
1.400
(Ln Z)^1/3

Fig.9.

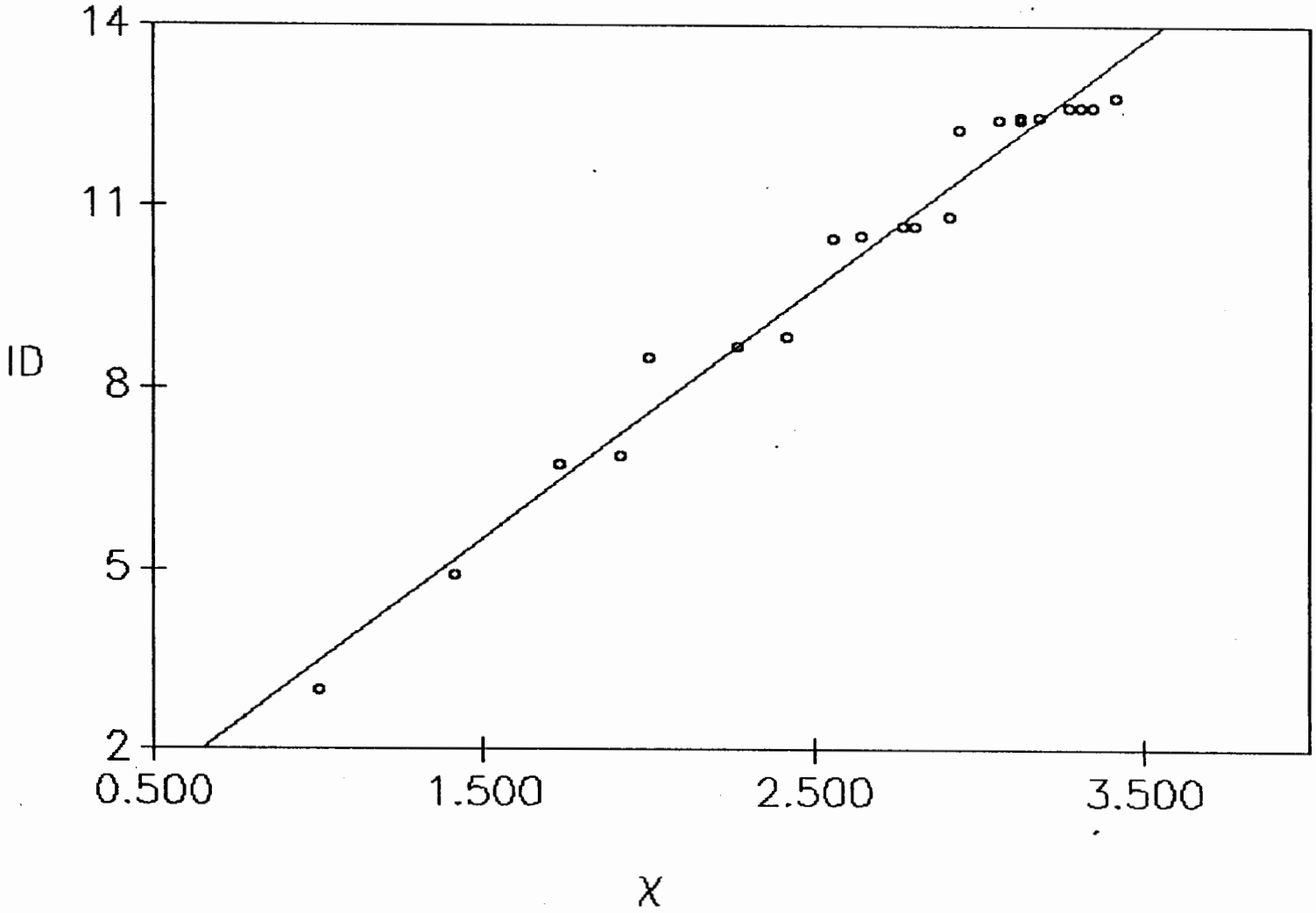


Fig.10.

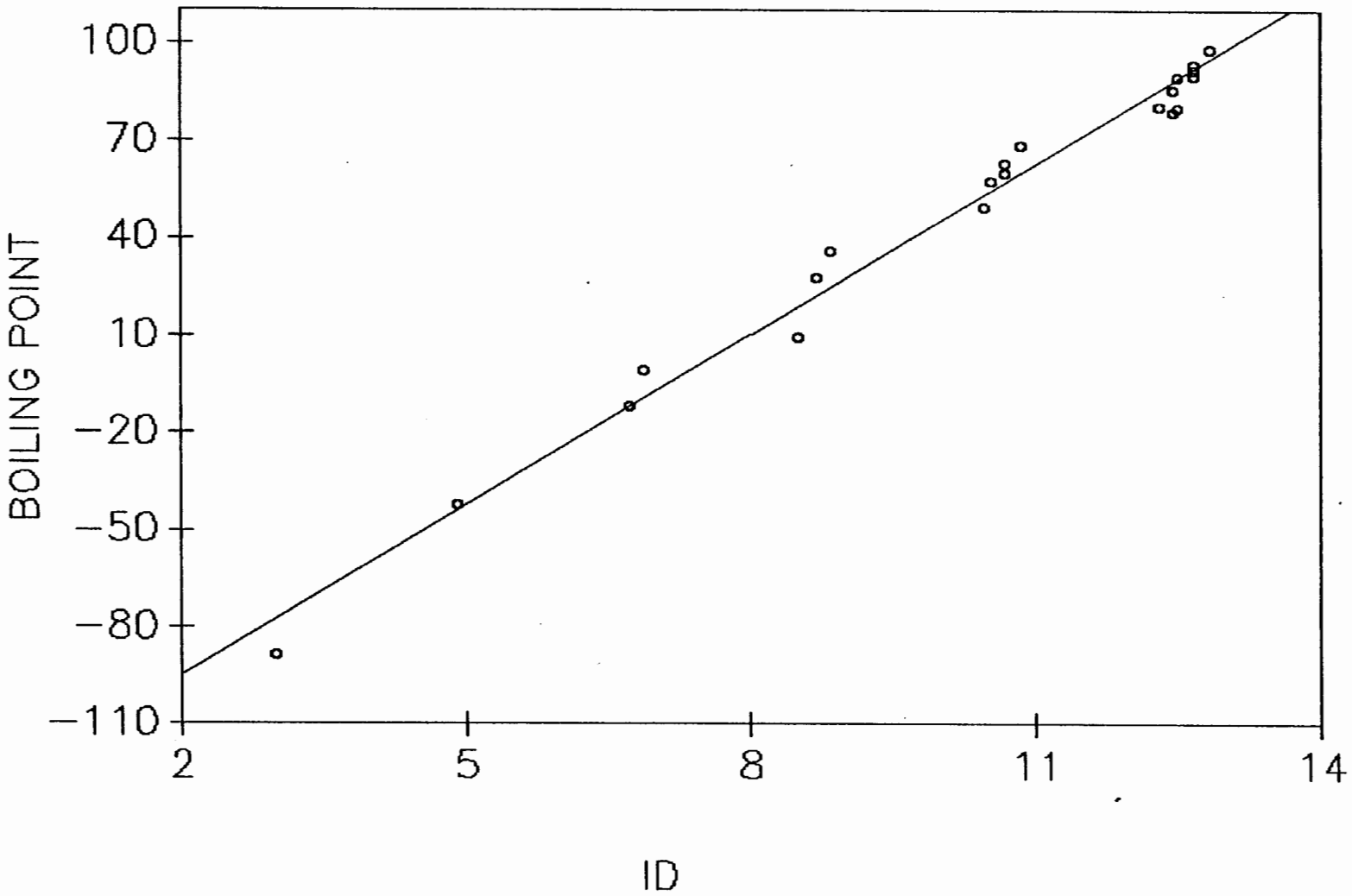
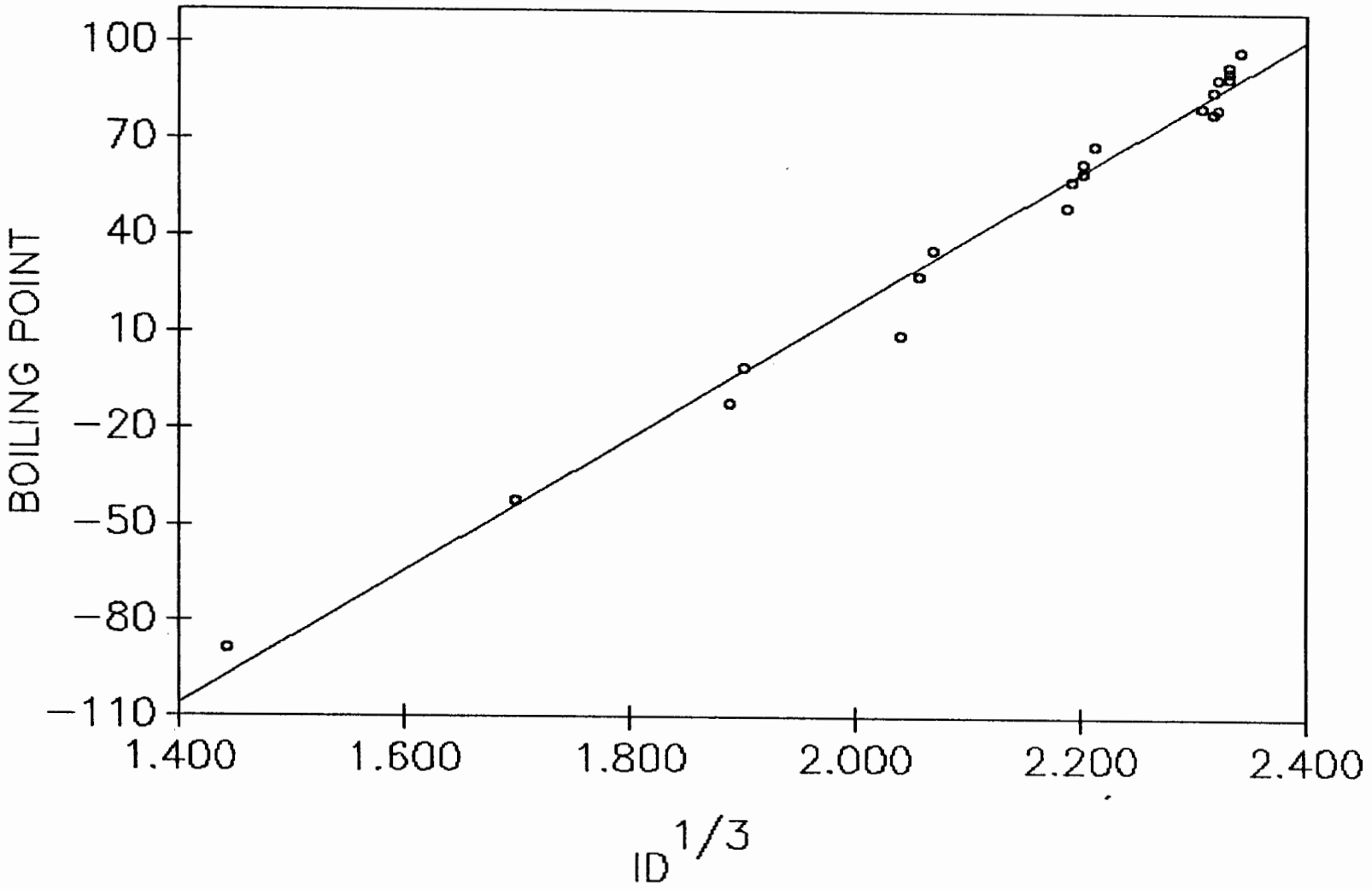


Fig.11.


100
70
40
10
−20
−50
−80
−110
BOILING POINT
1.400
1.600
1.800
2.000
2.200
2.400
ID 1/3