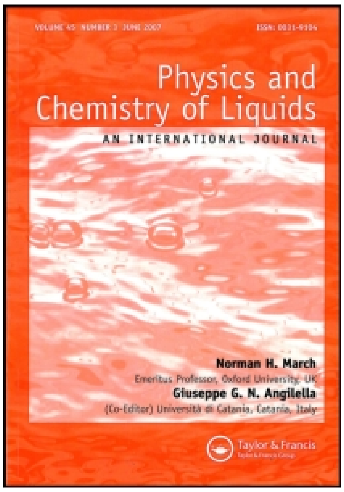

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A Prediction for the Critical Temperature of Organic Compounds from the Reduced Melting Temperature

J. AmorÓs[a]
[a] Departamento de Física Aplicada, Universidad de Cantabría, Santander, Spain

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A PREDICTION FOR THE CRITICAL TEMPERATURE OF ORGANIC COMPOUNDS FROM THE REDUCED MELTING TEMPERATURE

J. AMORÓS

Departamento de Física Aplicada, Universidad de Cantabría,
Avenida de Los Castros S/N, 39005, Santander, Spain

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The critical temperature T_c of organic chains has been predicted from the observed behaviour for the reduced melting temperature T_{rm}. For a number of carbon atoms sufficiently large, when the odd–even effect vanishes, T_{rm} reaches an approximately constant value, which changes very smoothly with the chain under consideration. Then the melting temperature T_m gives immediately a numerical value for T_c. If T_m is not known, T_c can be evaluated alternatively extrapolating the available values for the members of the chain.

Keywords: Critical temperature; Phase equilibria; Reduced melting temperature; Vaporization

1. INTRODUCTION

The critical temperature T_c is a quantity of basic importance both theoretically and experimentally. For low weight organic compounds the critical temperature is easily measured. When the mass increases, the critical temperature exceeds the temperature of the onset of thermal decomposition, thus impeding the measurement of the critical properties. Recently some methods of measuring critical properties of thermally unstable substances have been described [1,2]. There is, however, a limit to this procedure and the use of prediction methods for the determination of the critical temperature is unavoidable. Although there are excellent reviews [3,4] and monographies [5–7] with many data concerning this quantity, recent recopilations [8–13] and measurements [14–19] favour a revision of this matter.

The behaviour corresponding to the organic chains has been considered in detail. We have extended this study to the organic families whose experimental information allows the method to be applied in order to predict T_c for the following elements of the chain.

This prediction is based on the variation of the reduced melting temperature, like to the ratio between melting and critical temperatures, $T_{rm} = T_m/T_c$, with the number of carbon atoms n of the organic compound. For $n \leq 4$ this variation is frequently irregular. Then some families exhibit the well-known odd–even effect. The melting temperature of any even member is considerably higher than the averaged values of the two adjacent odd members. This peculiar behaviour is due to the distinct crystal structures describing the solid phase of all members. The n-alkanes (C_nH_{2n+2}) are the

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prototype of this phenomenon [20]. When *n* increases, this effect is clearly weakened until it practically disappears. From this chain length, T_{rm} is almost constant: $T_{rm} \approx C$ for the remaining range. This behaviour was assumed constant indefinitely so that critical temperature is given by $T_c = T_m/C$. Given that the melting temperature is frequently known, this simple relation allows critical temperature to be calculated. At the time, the values of T_{rm} are insufficient to reach stabilization. Then an extrapolation for T_c, if it is adequate, shows the expected behaviour. Such extrapolation can sometimes be utilized for the prediction of T_c when the data number for T_m is insufficient. However, this procedure does not allow T_{rm} to be determined, owing to the possible presence of the odd–even effect.

The organization of this paper is as follows. In the next section, results and discussion for T_c will be furnished. In the last section, the main conclusions to this work will be presented.

2. RESULTS AND DISCUSSION

We have selected 792 organic compounds whose data of T_m and T_c are known, and hence a value for T_{rm} can be determined. We have classified these compounds in ten large groups: 144 acyclic hydrocarbons, 161 cyclic hydrocarbons, 117 halogenated hydrocarbons, 60 sulphurated hydrocarbons, 14 acids, 108 alcohols, 32 esters, 40 alcanones and cetones, 35 alkanamines and 81 additional organic compounds. The complete results for T_{rm} are shown in Fig. 1. A high dispersion is observed not only globally but also in each group and even between isomers. This fact prevents the implantation of a general correlation except for the succesive elements of a chain. However, the majority of the compounds are included between 0.3 and 0.4. The extreme values are 0.742 for pentafluorophenol and 0.208 for 2-hexanethiol. In spite of these facts, a structural effect is remarkable. So, alcohols and halogenated hydrocarbons present a great value, due probably to the hydrogen bond in the first case and to the strongly polar bond in the second case. By the other hand, sulphurated and acyclic

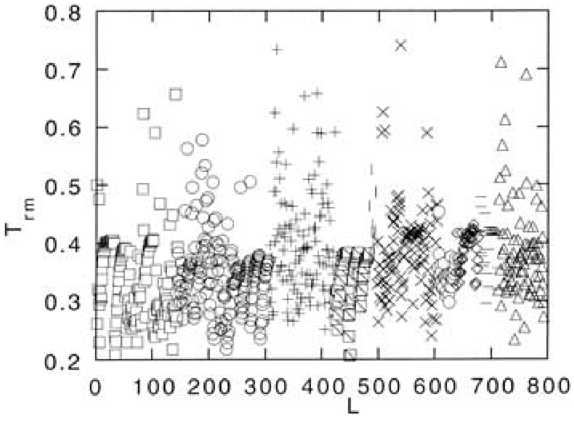

FIGURE 1 Variation of the reduced melting temperature T_{rm} for all the compounds analyzed: □ acyclic hydrocarbons; ○ cyclic hydrocarbons; + halogenated hydrocarbons; ⧅ sulphurated hydrocarbons; | acids; × alcohols; ⊙ esters; ◇ alkanones; - alkanamines; △ other organic compounds.

hydrocarbons present low values, although there are some exceptions. Next we consider the detailed study of each family.

(a) Alkanes, Alkenes and Alkines

Data for T_{rm} are available up to $n = 36$ (with some gaps) for alkanes [16] and up to $n = 20$ for alkenes and alkines [7] (Fig. 2). Clearly the behaviour of the three families converges towards a common value $T_{\mathrm{rm}} \approx 0.4$ when n increases. However, the effect odd–even is present in alkanes and alkines but not in alkenes. Additional data for T_{m} are available for alkanes up to $n = 100$ (with some gaps) [20,21] and for alkenes and alkines up to $n = 40$ [7]. Given that there are at least 20 values for T_{c}, we have fitted these points to an expression of the type:

$$T_{\mathrm{c}} = a + bn^{-1/2} + cn^{-1} + dn^{-3/2} + en^{-2} \tag{1}$$

This relation is highly satisfactory for alkanes. Obviously these parameters are not universal since they depend on the considered family. But in contrast T_{c} is determined immediately.

The fit was realized assigning distinct weights to the data considering $n \geq 5$. The coefficients of the fit, the maximum absolute deviation (MAD), the average absolute deviation (AAD) and the percentage average deviation (PAD), defined as $100 \sum |T_{\mathrm{c}}^{\mathrm{dat}} - T_{\mathrm{c}}^{\mathrm{calc}}| / T_{\mathrm{c}}^{\mathrm{dat}}$ are the following:

alkanes: $a = 1123.0$; $b = -619.90$; $c = -8666.5$; $d = 23554$; $e = -18739$; MAD $= 7.446$; AAD $= 1.307$; PAD(%) $= 0.1680$.
alkenes: $a = 1232.2$; $b = -2025.8$; $c = -2012.2$; $d = 9855.2$; $e = -8509.6$; MAD $= 4.482$; AAD $= 1.223$; PAD(%) $= 0.1721$.

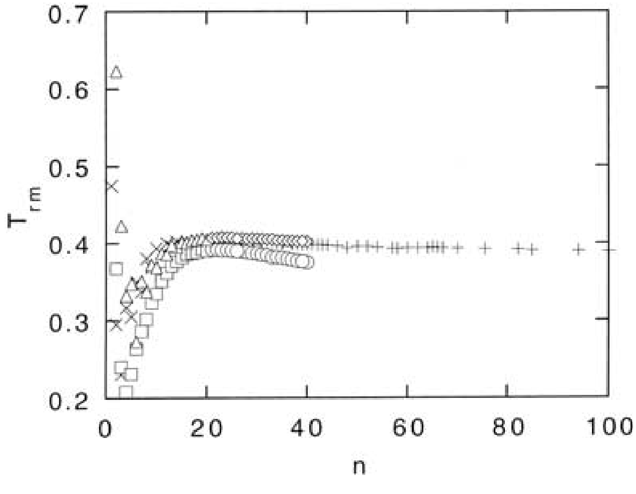

FIGURE 2 Reduced melting temperature T_{rm} *versus* number of carbon atoms n: × available values for alkanes; + extrapolated values for alkanes; □ available values for alkenes; ○ extrapolated values for alkenes; △ available values for alkines; ◇ extrapolated values for alkines.

alkines: $a=1510.0$; $b=-5604.6$; $c=14222$; $d=-21406$; $e=13695$; MAD = 1.285; AAD = 0.3758; PAD(%) = 0.05385.

Figure 2 also includes the presence of the additional points arising from the fit. The result confirms the predictions. The constant C holds 0.404, 0.392 and 0.406 for alkanes, alkenes and alkines respectively.

(b) Diphenylalkanes, Alkylbenzenes, Alkylcyclohexanes and Alkylcyclopentanes

The existent range [7] is $n=13$–28 for T_m and T_c of diphenylalkanes; $n=6$–22 for T_c and also $n=23$–42 for T_m of normal alkylbenzenes and normal alkylcyclohexanes, and $n=5$–21 for T_c and also $n=22$–41 for T_m of normal alkylcyclopentanes. Figure 3 presents the results for the four groups. In the case of diphenylalkanes, the odd–even effect persists as far as the last point available. However the limit for T_{rm} can be estimated as $C=0.36$. This effect is practically absent in the remaining families. The extrapolation for T_c is also possible. Excepting the diphenylalkanes, such extrapolation allows the values of T_{rm} to be increased. The common limit for T_{rm} is approximately $C=0.40$, 0.38 and 0.37 for the three involved families.

The coefficients of the Eq. (1) are:

diphenylalkanes: $a=4505.0$; $b=-66770$; $c=467640$; $d=-1473700$; $e=1731900$; MAD = 1.643; AAD = 0.5614; PAD(%) = 0.07042.
normalalkylbenzenes: $a=842.26$; $b=3103.4$; $c=-26058$; $d=61110$; $e=-49032$; MAD = 1.073; AAD = 0.1926; PAD(%) = 0.02888.
normalalkylcyclohexanes: $a=1693.2$; $b=-8970.8$; $c=37672$; $d=-87371$; e=7877; MAD = 2.302; AAD = 0.5179; PAD(%) = 0.08111.
normalalkylcyclopentanes: $a=1792.7$; $b=-9765.8$; $c=38065$; $d=-79318$; $e=64174$; MAD = 3.164; AAD = 0.8054; PAD(%) = 0.1311.

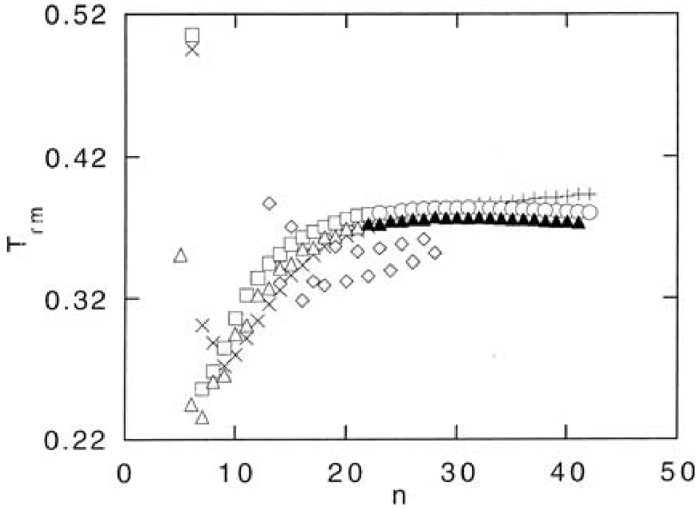

FIGURE 3 As for Fig. 2: ◇ available values for diphenylalkanes; × available values for alkylbenzenes; + extrapolated values for alkylbenzenes; □ available values for alkylcyclohexanes; ○ extrapolated values for alkylcyclohexanes; △ available values for alkylcyclopentanes; ▲ extrapolated values for alkylcyclopentanes.

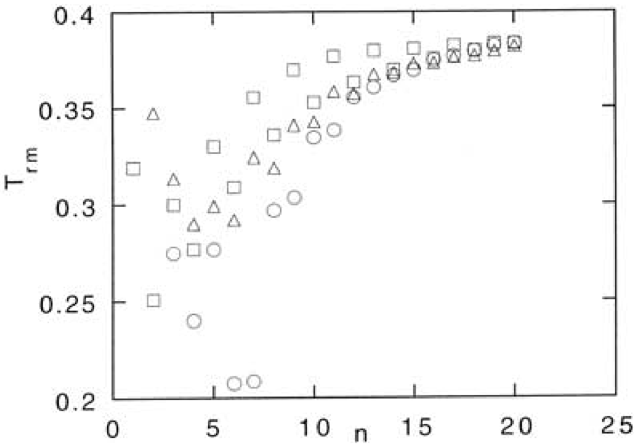

FIGURE 4 Available values for T_{rm}: □ 1-Alkanethiols; ○ 2-Alkanethiols; △ 2-Thiaalkanes.

(c) 1-Alkanethiols, 2-Alkanethiols and 2-Thiaalkanes

The available range [7] is for T_m and T_c, $n = 1$–20, $n = 3$–20 and $n = 2$–20 for 1-alkanethiols, 2-alkanethiols and 2-thiaalkanes respectively. Figure 4 shows the results obtained. The odd–even effect is appreciable for the first and third groups but not for the second. The T_{rm} data present an almost perfect convergence for the greater values of n in all cases. This common limit can be fixed as $C = 0.383$. Higher values of T_c are accesible only by means of the extrapolation. Applying the usual expression, we obtain:

1-alkanethiols: $a = 1226.0$; $b = -2491.5$; $c = 3178.3$; $d = -1873.8$; $e = 431.04$;
MAD = 1.246; AAD = 0.3254; PAD(%) = 0.05105.
2-alkanethiols: $a = 1104.6$; $b = -992.65$; $c = -3543.3$; $d = 10370$; $e = -7451.2$;
MAD = 1.486; AAD = 0.4149; PAD(%) = 0.06422.
2-thiaalkanes: $a = 1121.6$; $b = -1295.7$; $c = -1658.2$; $d = 5909.9$; $e = -3849.2$;
MAD = 5.363; AAD = 0.9849; PAD(%) = 0.1605.

(d) 1-Fluoroalkanes, 1,1-Difluoroalkanes and 1,1,1-Trifluoroalkanes

T_c values [7] exist in the range $n = 3$–20, $n = 3$–20 and $n = 2$–20 for 1-fluoroalkanes, 1,1-difluoroalkanes and 1,1,1-trifluoroalkanes respectively. T_m values are, however, absent. Therefore only an extrapolation allows to obtain higher values for T_c. A fit according to (1) gives:

1-fluoroalkanes: $a = 1290.7$; $b = -3177.7$; $c = 3905.1$; $d = -1581.0$; $e = -315.68$;
MAD = 0.1923; AAD = 0.09161; PAD(%) = 0.01493.
1,1-difluoroalkanes: $a = 1356.5$; $b = -4038.5$; $c = 7778.6$; $d = -8958.1$; $e = 4825.5$;
MAD = 0.4689; AAD = 0.1852; PAD(%) = 0.03153.
1,1,1-trifluoroalkanes: $a = 1242.1$; $b = -2633.4$; $c = 1352.7$; $d = 2522.9$; $e = -2407.5$;
MAD = 2.669; AAD = 0.5071; PAD(%) = 0.1023.

(e) *n*-Alkyl Metanoates, Etanoates, Propanoates, Butanoates and Pentanoates

T_c values are available [7] in the range $n = 2$–21, $n = 3$–22, $n = 4$–23, $n = 5$–24 and $n = 6$–25 for n-alkyl metanoates, etanoates, propanoates, butanoates and pentanoates respectively, whereas T_m. values are non-existent. Therefore T_{rm} can be not evaluated. The distribution obtained allows a global fit for all the families with the following result:

$a = 1137.7$; $b = -1415.5$; $c = -2389.0$; $d = 8472.8$; $e = -5805.1$; MAD = 11.88;
AAD = 2.577; PAD(%) = 0.4069.

Although this result is acceptable, a specific fit for each family would appreciably improve the prediction. This is specially advisable because the test of T_{rm} is not possible.

We can then present the results corresponding to each group.

n-alkyl metanoates: $a = 1201.3$; $b = -2333.6$; $c = 2021.9$; $d = 414.02$; $e = -885.59$;
MAD = 1.722; AAD = 0.2527; PAD(%) = 0.04445.
n-alkyl etanoates: $a = 1230.1$; $b = -2717.6$; $c = 3896.9$; $d = -4011.7$; $e = 2868.5$;
MAD = 2.153; AAD = 0.2820; PAD(%) = 0.04656.
n-alkyl propanoates: $a = 1174.9$; $b = -2091.6$; $c = 1880.8$; $d = -2669.9$; $e = 4240.0$;
MAD = 0.9638; AAD = 0.1583; PAD(%) = 0.02589.
n-alkyl butanoates: $a = 1142.4$; $b = -1812.0$; $c = 1543.4$; $d = -4847.0$; $e = 8680.9$;
MAD = 0.8420; AAD = 0.1719; PAD(%) = 0.02589.
n-alkyl pentanoates: $a = 1188.0$; $b = -2685.2$; $c = 7705.7$; $d = -23390$; $e = 28606$;
MAD = 0.8385; AAD = 0.1513; PAD(%) = 0.02198.

(f) Alkanoic Acids

T_c values are available for $n = 1$–10 [15], whereas T_m data exist for $n = 1$–20 and $n = 22,24,26,28$–30 and 32 [5,22–25]. The odd–even effect is clearly appreciable in the experimental range (Fig. 5). The fit results for T_c. give:

$a = 1107.6$; $b = -1547.2$; $c = 701.01$; $d = 1440.6$; $e = -1122.0$; MAD = 1.740;
AAD = 0.6335; PAD(%) = 0.09454.

Extending the results for T_{rm} with these data, we appreciate the presence of the odd–even effect up to $n \approx 20$ and later T_{rm} takes a approximately constant value $C = 0.42$.

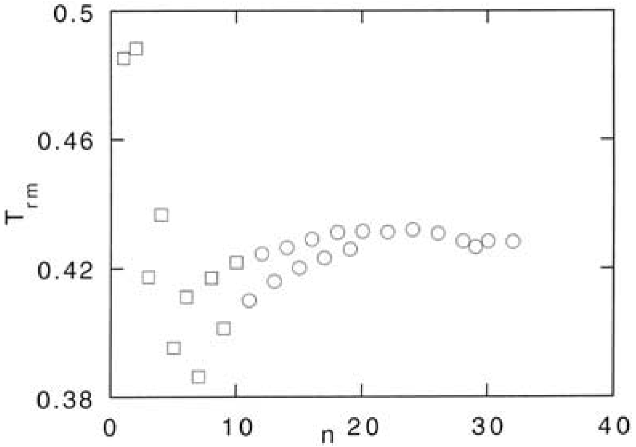

FIGURE 5 As for Fig. 2 for alkanoic acids: □ available values; ○ calculated values.

(g) Alkanols

T_c values for 1-alkanols in the range $n = 1$–20 and 22 have been supplied recently [11,17], and T_m values are also available [6,21]. Here the odd–even effect is practically non-existent (Fig. 6). We have extrapolated the T_c values according to (1) for $n \geq 3$ and assigning different weights to the experimental points [17]. The numerical values are:

$a = 1390.4$; $b = -3824.5$; $c = 6568.1$; $d = -5224.9$; $e = 1536.2$; MAD = 2.503;
AAD = 0.5472; PAD(%) = 0.07509.

Figure 6 also shows a stabilization for $T_{rm} = C = 0.41$.

T_c and T_m values for 2-alkanols are available up to $n = 20$ [6,7,11]. The odd–even effect is clearly present but the last points suggest the stabilization around $T_{rm} = C = 0.42$ (Fig. 6). The coefficients of the Expression (1) are:

$a = 1262.4$; $b = -2286.6$; $c = -311.15$; $d = 7051.0$; $e = -6185.0$; MAD = 7.713;
AAD = 1.658; PAD(%) = 0.2271.

T_c values for 3-alkanols are scarce ($n = 5$–10) [11] but T_m values are more numerous ($n = 5$–18 with some exceptions) [6]. Owing to the few points existent for T_c, it is advisable to diminish the number of coefficients in the fit. Eliminating the last coefficient in (1), we find:

$a = 911.95$; $b = 164.48$; $c = -5024.9$, $d = 6474.8$; MAD = 0.4727; AAD = 0.2491;
PAD(%) = 0.04022.

The odd–even effect is not visible although the numerical data are scarce. Figure 6 shows the result obtained which makes possible a limit for T_{rm} between 0.42 and 0.43.

Figure 7 presents the variation of critical temperature T_c *vs* the order number N of alkanols ($N = 1$–5). It is evident that the T_c for 1-alkanols is clearly higher than the remainder with the same n but later the variation is very smooth suggesting that the T_c of the last known element is a good prediction for the following ones.

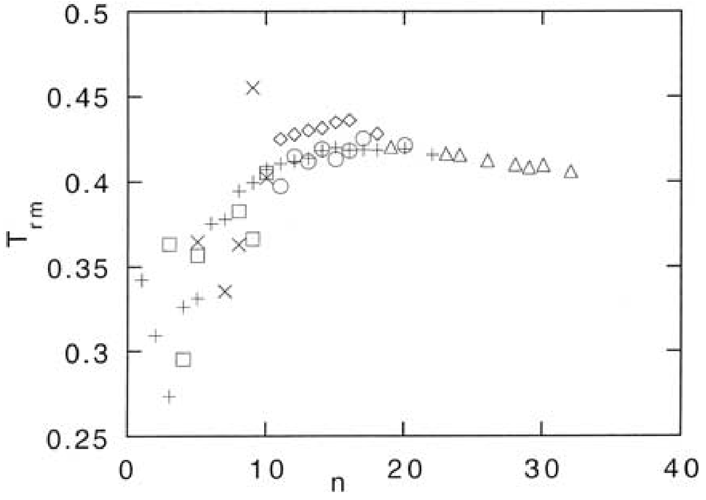

FIGURE 6 As for Fig. 2 for 1-alkanols: + available values, △ extrapolated values; for 2-alkanols: □ available values, ○ extrapolalated values; for 3-alkanols: × available values, ◇ extrapolated values.

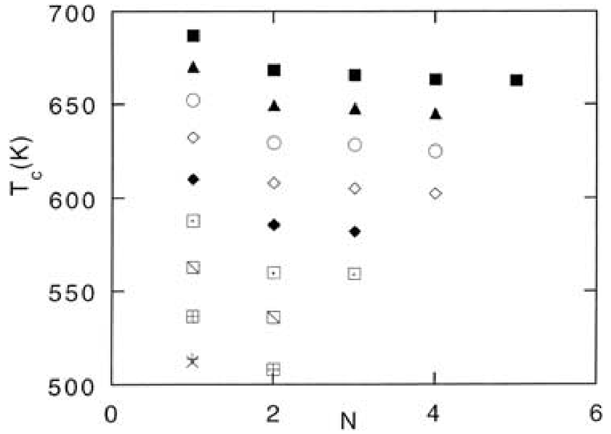

FIGURE 7 Critical temperature T_c *versus* order number N for N-alkanols: × metanol, + etanol; ⊞ propanols; ⧅ butanols; ⊡ pentanols; ◆ hexanols; ◇ heptanols; ○ octanols; ▲ nonanols; ■ decanols.

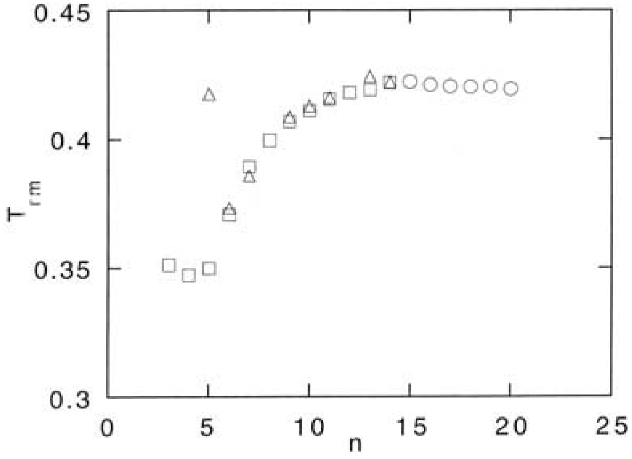

FIGURE 8 As for Fig. 2 for 2-alkanones: □ available values, ○ extrapolated values; and for 3-alkanones: △ available values.

(h) *n*-Alkanones

T_m and T_c values are available for $n = 3$–20 [6] and $n = 3$–14 [14] in the case of 2-alkanones. A fit allows an extrapolation for T_c values up to $n = 20$. The coefficients of this fit are:

$a = 823.46$; $b = 1792.3$; $c = -14170$; $d = 27591$; $e = -17428$; MAD = 0.9233;
AAD = 0.4246; PAD(%) = 0.0659.

The odd–even effect is absent and T_{rm} tends towards approximately 0.42 (Fig. 8).

For 3-alkanones we have T_m and T_c values in the range $n = 5$–14 [6,14]. We can extrapolate T_c with our usual formula. The results are:

$a = 200.53$; $b = 9456.1$; $c = -48603$; $d = 94377$; $e = -64740$; MAD = 1.191;
AAD = 0.3950; PAD(%) = 0.05915.

However, it is not possible extrapolate T_{rm}. Figure 8 shows a behaviour practically coincident with that of 2-alkanones.

For 4-alkanones we have T_c values in the range $n = 7$–14 [14], but a minor range for T_m, [6]. Therefore a prediction for T_{rm}, is not feasible but the extrapolation for T_c is even possible with the following result: $a = 128.74$; $b = 11396$; $c = -62255$; $d = 131020$; $e = -98721$; MAD = 0.2930; AAD = 0.1531; PAD(%) = 0.02306.

For 5-alkanones, 6-alkanones and 7-alkanones, T_c values are available for $n = 9$–13, $n = 11$–13 and $n = 13$–14 respectively [14]. Evidently no conclusion is possible.

However, the similarity observed globally suggests a fit including all n-alkanones. The resulting parameters are as follows:

$a = 1248.7$; $b = -2337.0$; $c = 209.57$; $d = 6044.3$; $e = -5614.9$; MAD = 6.495;
AAD = 2.714; PAD(%) = 0.4064.

The variation of the critical temperature vs. the order number N of alkanones reveals a smooth decrease for all values of n (Fig. 9).

(i) Alkanamines

T_m and T_c values are available for 1-alkanamines [5,7] in the range $n = 1$–20. The odd–even effect persists as far as the mentioned limit (Fig. 10). However, this plot shows a convergence between 0.41 and 0.42. Alternatively, the extrapolation of T_c by means of Eq. (1) provides the following results:

$a = 1269.5$; $b = -2840.2$; $c = 3675.3$, $d = -2151.2$; $e = 476.66$; MAD = 3.227;
AAD = 0.5399; PAD(%) = 0.03357.

On the other hand, only T_c values are available [7] for N-methyl-1-alkanamines ($n = 2$–20), N-ethyl-l-alkanamines ($n = 5$–20), N-alkyl-1-alkanamines ($n = 4$–20, only even values) and N,N-dimethyl-l-alkanamines ($n = 3$–20). Figure 11 shows the existent data. For $n \geq 5$ there is an appreciable agreement for the values of the four families.

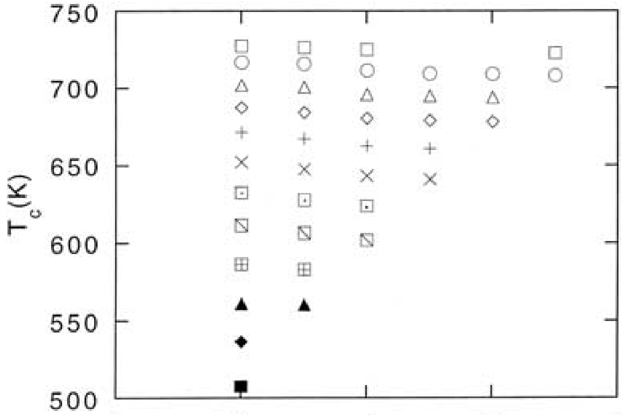

FIGURE 9 As for Fig. 7 for N-alkanones: ■ propanone; ◆ butanone; ▲ pentanones; ⊞ hexanones; ⧅ heptanones; ⊡ octanones; × nonanones; + decanones; ◇ undecanones; △ dodecanones; ○ tridecanones; □ tetradecanones.

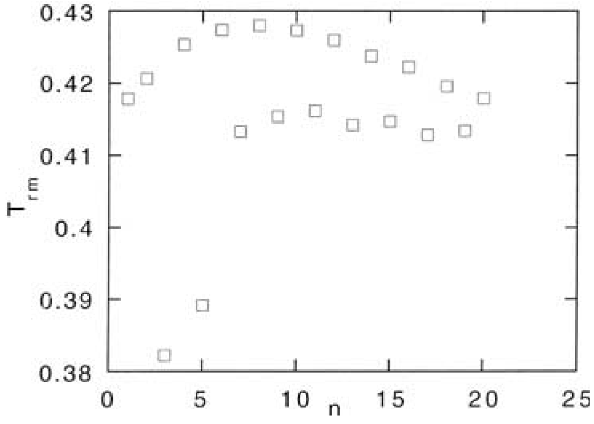

FIGURE 10 As for Fig. 2 for 1-alkanamines: □ available values.

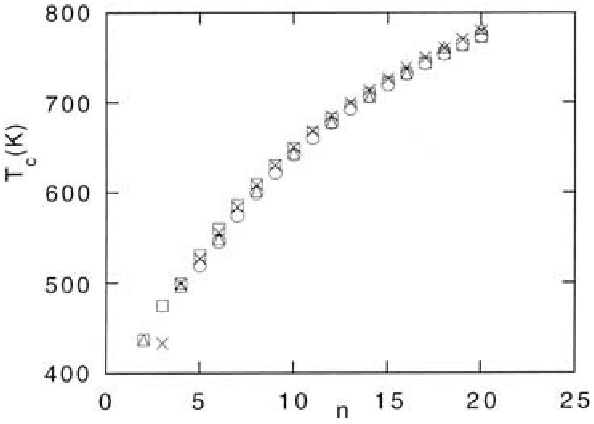

FIGURE 11 Critical temperature T_c *versus* carbon atoms number *n*: □ *N*-methyl-1-alkanamines; ○ *N*-ethyl-1-alkanamines; △ *N*-alkyl-1-alkanamines; × *N*,*N*-dimethyl-l-alkanamines.

Additional values for T_c are only feasible for all compounds by means of the extrapolation. The results of the usual fit are:

N-methyl-l-alkanamines: $a = 1153.4$; $b = -1711.0$; $c = -1054.7$; $d = 5822.3$; $e = -4149.1$; MAD = 2.694; AAD = 0.6103; PAD(%) = 0.1060.
N-ethyl-1-alkanamines: $a = 1376.0$; $b = -4339.6$; $c = 10761$, $d = -18394$; $e = 14438$; MAD = 0.4586; AAD = 0.1687; PAD(%) = 0.02682.
N-alkyl-l-alkanamines: $a = 1449.0$; $b = -4417.9$, $c = 7784.8$; $d = -6697.8$; $e = 2351.3$; MAD = 3.207; AAD = 1.539; PAD(%) = 0.2346.
N,*N*-dimethyl-l-alkanamines: $a = 853.63$; $b = 2181.7$; $c = 18877$; $d = 40478$; $e = -28595$; MAD = 2.578; AAD = 0.8344; PAD(%) = 0.1394.

Lastly, we have also made a fit including the four families for $n \geq 5$ with the following result:

$a = 1583.4$; $b = -6814.0$; $c = 21571$; $d = 38617$ $e = 28253$; MAD = 7.014; AAD = 3.360; PAD(%) = 0.5187.

3. CONCLUSION

Our study attempts to furnish a simple method for the prediction of the critical temperature of organic chains. Furthermore, an extrapolation of this quantity makes a complementary evaluation possible, which is the only procedure possible when the T_m data are not available.

Our method also makes it possible to analyze the existence of the odd–even effect. Although this effect is founded on structural considerations, it is apparently surprising that related families show distinct behaviour with relation to its presence.

The limit for T_{rm}, when n increases, is well-established in a narrow range between 0.36 and 0.43. However, this value seems sensitive to the involved family. Thus, the minor values (up to $n = 0.40$) correspond to the hydrocarbons and its sulphurated derivatives. In contrast, the higher values correspond to the nitrogen compounds and mainly to the oxygen compounds. Here the differences between related families are small.

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