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Thermal analysis of some novel pyrimidine derivatives

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Summary

Some new pyrimidine derivatives have been synthesized and their decomposition characteristics have been studied by thermogravimetric and differential scanning calorimetric analysis. The thermal stability and some kinetics parameters of decomposition were evaluated from thermograms. It is observed that depending upon the structure, substitutions, thermal stability and decomposition kinetics varies in different compounds.

Key words: Thermal gravimetric analysis, differential scanning calorimetry, thermal stability, kinetic parameters.

Resumen

Análisis térmico de algunos nuevos derivados de pirimidina

Se sintetizaron algunos nuevos derivados de pirimidina y se estudiaron sus características de descomposición mediante análisis termogravimétrico y calorimétrico diferencial de barrido. La estabilidad térmica y algunos parámetros cinéticos de descomposición se evaluaron a partir de los respectivos termogramas. Se observa que, dependiendo de la estructura y las sustituciones, la estabilidad térmica y la cinética de descomposición varían entre los diferentes compuestos.

Palabras clave: análisis termogravimétrico, calorimetría diferencial de barrido, estabilidad térmica, parámetros cinéticos.

Introduction

Thermal analysis has been used to determine the physical and chemical properties of various types of materials [1-6]. Scientific and technological achievements together with demands based on industrial requirement have permitted the development of various types of materials that can withstand at much higher temperatures and more corrosive environments. It is widely used in various fields to study composition analysis, product reliability, stability, chemical reaction and dynamic properties [7-9]. The analysis is popular in various industries namely pharmaceutical [10, 11], forensic [12, 13], food [14, 15], ceramics [16, 17], polymer [18, 19], composites [20, 21] and semiconductors [22] industries. Further, by thermal analysis, kinetic parameters of thermally simulated reactions can be evaluated which provides a deeper insight in to the mechanism of high energetic compounds [23-26].

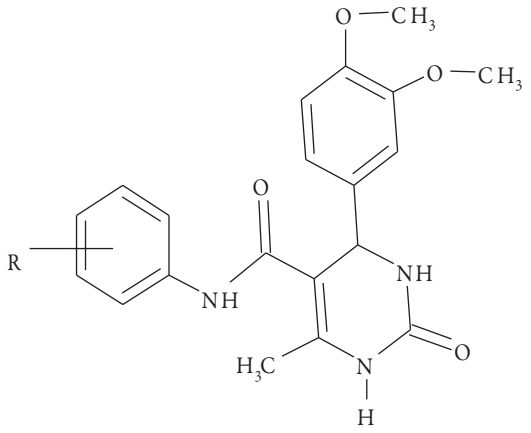
Literature survey shows that thermal analysis has been reported for a variety of materials such as coals, rocks, minerals, nano-materials, rubber, styrene butadiene blends, polyimide resins, superconducting materials, hydrogen storage materials, rocks from moon, hydrocarbon sludge etc. [27-30]. Thermal analysis can be done by various techniques such as differential scanning calorimetry, differential thermal analysis, thermogravimetric analysis, evolved gas detection, evolved gas analysis etc.

Among many heterocyclic compounds, pyrimidine compounds are one of the most prominent structures which attract many chemists and pharmacists due to their therapeutic values. Further, many of these compounds are known to exist in deoxyribonucleic acid and ribonucleic acid which is one of the most essential constituents of all cells and thus of all living matter. As many of these compounds exist in various drugs [31-33], it would be useful to study their thermal stability and other thermal parameters which are prime factors for the application and shelf life of a drug.

Thus, in the present work, thermal properties of some newly synthesized pyrimidine derivatives such as dihydropyrimidinones, dihydropyrimidinthiones, tetrahydropyrimidines and 2, 4-disubstituted pyrimidines have been studied by thermogravimetric (TG) and differential scanning calorimetric (DSC) techniques. From TG thermograms, the thermal stability and various kinetic parameters such as order of the degradation, energy of activation, frequency factor and entropy change have been evaluated. The purity of synthesized compounds has been checked by DSC which also gives the melting points and heat of fusion of the studied compounds.

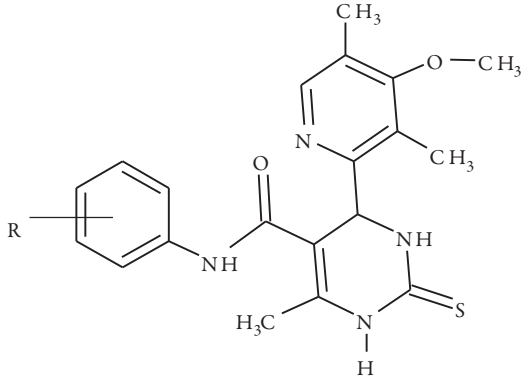
Experimental

A wide variety of pyrimidine compounds have been synthesized. The general structures and substitutions in different compounds are given in Figure 1.



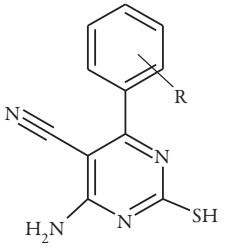
Where R is:

SNO-1: 4-OCH_3; SNO-2: 4-CH_3; SNO-3: 4-Cl; SNO-4: 2-CH_3; SNO-5: 3-OCH_3; SNO-6: 4-F; SNO-7: 2,5-diCl; SNO-8: 3-Cl; SNO-9: 3, 4-Cl; SNO-10: 3-Cl, 4-F;



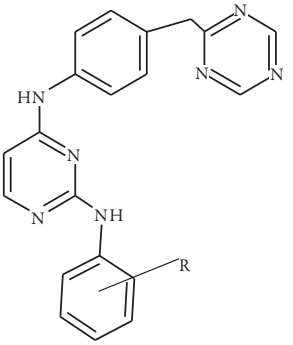
Where R is:

SSN-1: 4-OCH_3; SSN-2: -H; SSN-3: 4-CH_3; SSN-4: 4-F; SSN-5: 4-OH; SSN-6: 3-Cl; SSN-7: 3-NO_2; SSN-8: 2-Cl; SSN-9: 2-NO_2; SSN-10: 2-OH;

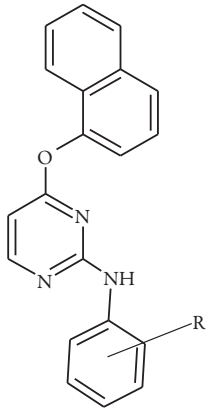


Where R is:

SNS-1: 4-OH, 3-OCH_3-C_6H_4; SNS-2: 4-OCH_3-C_6H_4; SNS-3: 4-OH-C_6H_4; SNS-4: 4-Cl-C_6H_4; SNS-5: 3-Cl-C_6H_4; SNS-6: 4-F-C_6H_4; SNS-7: 3-NO_2-C_6H_4; SNS-8: -C_6H_5; SNS-9: C_4H_3O; SNS-10: -CH=CH-C_6H_5;



Where R is: SDN-1: 4-Cl; SDN-2: 4-CH_3; SDN-3: 4-F; SDN-4: 3-CF_3; SDN-5: 3-Cl, 4-F;



Where R is: SDO-1: 4-Cl; SDO-2: 4-CH_3; SDO-3: 4-F; SDO-4: 3-CF_3; SDO-5: 3-Cl, 4-F

Figure 1. General structure of synthesized different pyrimidine derivatives.

Thermal analysis

Thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) measurements were made using instrument "Pyris-1, Perkin Elmer Thermal analysis" at the heating rate of 10°C/min in nitrogen atmosphere for all the synthesized compounds.

Results and discussion

Thermal stability

Figure 2 shows the TGA thermogram of a single pyrimidine compound SSN-1. Various thermal properties such as decomposition temperature range, percentage weight loss and residual weight are reported in table 1 for all the compounds.

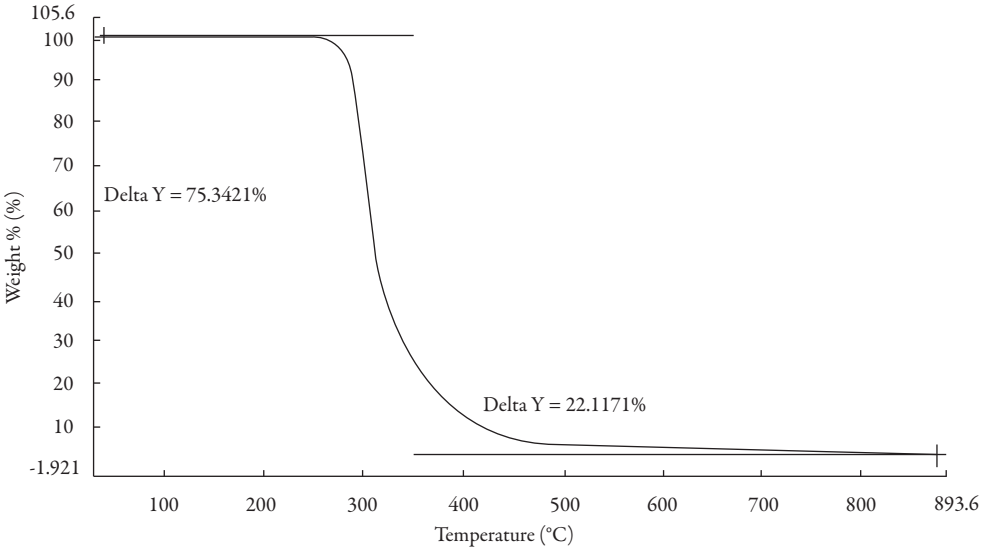


Figure 2. The TGA graphs of SSN-1.

SNO series.

For some compounds, degradation is single step process whereas for others, it is multi step process. For SNO-1 and SNO-3, degradation is multi step process whereas for other compounds, it is single step. Table 1 show that SNO-9 and SNO-10 is most unstable and SNO-6 and SNO-8 are stable. As evident from Figure 1, substitutions are different in different compounds although central moiety is same. SNO-10 contains 3-chloro and 4-fluoro groups whereas SNO-9 has two chloro groups at 3 and 4 positions. SNO-6- contains 4-fluoro group whereas SNO-8 contains only 3-chloro group.

Thus, the number and position of group also affect the stability of compound. Other compounds containing different other substitutions have intermediate thermal stability.

Table 1. TGA data for synthesized compounds.

Comp. Code	Amount (mg)	Decomposition Range (°C)	% Weights loss	Residual wt. loss (mg)
SNO Series				
SNO-1	0.933	150-700	97.96	0.913
SNO -2	2.714	170-550	90.69	2.461
SNO -3	3.247	165-480	59.86	1.943
SNO -4	2.527	175-450	58.81	1.481
SNO -5	2.616	145-510	58.85	1.539
SNO -6	9.477	210-610	57.33	5.433
SNO -7	7.571	150-380	84.05	6.363
SNO -8	4.175	210-485	72.50	3.026
SNO -9	5.834	100-500	75.37	4.396
SNO -10	8.559	100-490	52.01	4.472
SSN Series				
SSN-1	2.230	188-621	99.74	2.222
SSN -2	5.827	280-792	98.75	5.754
SSN -3	1.490	255-824	98.80	1.472
SSN -4	2.727	230-665	99.21	2.705
SSN -5	2.916	167-820	81.76	2.384
SSN -6	4.922	125-548	86.24	4.244
SSN -7	9.423	200-600	61.31	5.777
SSN -8	7.493	178-400	79.74	5.974
SSN -9	4.406	146-400	65.44	2.883
SSN -10	5.800	98-500	64.94	3.766

(Continued)

Table 1. TGA data for synthesized compounds.

Comp. Code	Amount (mg)	Decomposition Range (°C)	% Weights loss	Residual wt. loss (mg)
SNS Series				
SNS-1	5.285	168-311	95.55	5.050
SNS-2	4.614	133-281	96.36	4.446
SNS-3	0.912	159-281	94.76	0.8642
SNS-4	6.505	100-200	97.24	6.326
SNS-5	4.009	83-161	97.50	3.909
SNS-6	3.401	125-234	99.34	3.378
SNS-7	2.103	169-287	64.55	1.3575
SNS-8	2.734	123-233	98.46	2.692
SNS-9	2.105	97-205	99.07	2.086
SNS-10	2.656	78-418	64.48	1.7125
SDN Series				
SDN-1	3.361	80-800	88.16	2.963
SDN-2	4.716	105-735	98.79	4.665
SDN-3	2.360	110-630	96.59	2.279
SDN-4	2.856	140-680	97.96	2.798
SDO Series				
SDO-1	2.791	90-635	98.53	2.750
SDO-2	1.513	120-600	96.69	1.463
SDO-3	1.765	90-525	88.44	1.561
SDO-4	2.961	95-530	96.00	2.842
SDO-5	2.907	105-610	95.54	2.777

SSN series.

For most of these compounds, degradation is single step process. However, for compounds SSN-1 and SSN-6, multi-step degradation takes place. It is clear from Table 1 that SSN-10 is most unstable and SSN-2 is most stable. SSN-10 contains 2-OH group

whereas SSN-2 is without substitution. Thus, the absence of any functional group to aryl ring increases the stability. The decomposition continues up to approximately 800 and up for SSN-2, SSN-3 and SSN-4. SSN-2 is without any functional group. SSN-3 and SSN-4 contain 4-methyl and 4-fluoro groups respectively which increase the decomposition temperature. Comparison of SSN-5 and SSN-10 shows that SSN-5 is more stable than SSN-10. Both these compounds contain hydroxyl group. In SSN-5, it is at 4^{th} position whereas in SSN-10, it is at 2^{nd} position. Similarly, SSN-6 and SSN-8 contain chloro group at 3^{rd} and 2^{nd} positions respectively. However, the decomposition temperature range for these compounds is different. In SSN-7 and SSN-9 compounds, nitro group is present at 4^{th} and 2^{nd} positions respectively. In this case, SSN-9 is unstable than SSN-7. Again, decomposition range is higher for SSN-7 containing 3-nitro group. This suggests that position of functional groups also affect the stability and the presence of group at 2^{nd} position decreases the stability.

SNS series.

For all the compounds, degradation is single step process and degradation temperature is less than 200 °C. Out of ten compounds, SNS-10 is most unstable which is followed by SNS-5. SNS-7 is the most stable compound which is followed by SNS-1. SNS-10 contains cinnamaldehyde as substitution to aromatic ring. Thus, cinnamaldehyde decreases the thermal stability. The presence of nitro group at 3^{rd} position increases the stability as in SNS-7. The variation in thermal decomposition may also be due to some intermolecular interactions (structural as well as electronic).

SDN series.

For all the compounds, degradation is multi step process. It is clear from Table 1 that for SDN series compounds, SDN-1 is most unstable and SDN-4 is most stable compound. SDN-4 contains 3-CF_3 whereas SDN-1 contains 4-chloro substitution. Thus, substitution affects the thermal stability of a compound. Overall, the dominating effect of different group is: positive resonating (+R) > positive hyper conjugation effect (+H) > negative inductive (-I). In the present study, order of effect of different substitution is 4-Cl > 4-CH_3 > 4-F> 3-CF_3. The more stability of SDN-4 may be due to negative inductive effect of 3-CF_3. Whereas due to positive resonating effect of 4- CH_3 group, SDN-1 is most unstable.

SDO series.

Table 1 shows that SDO-2 is most stable while SDO-1 and SDO-3 are unstable. Thus, the presence of 4-CH_3 group increases the stability. SDO-1 and SDO-3 contain 4-chloro and 4-fluoro group respectively which causes decrease in stability. However,

when a compound contains both chloro and fluoro groups as in SDO-5, stability increased.

Comparison of SDN and SDO series suggests that structure affects decomposition. The central moieties are different in both series but side chains are same. In SDN series, 3-CF_3 increased the stability whereas in SDO series, it decreased the stability.

Overall comparison of synthesized compounds shows that a substitution in a particular moiety increases thermal stability whereas the same substitution in other moiety causes decrease of stability. This suggests that the variation in thermal decomposition may also be due to some intermolecular interactions.

Kinetic parameters

Further, from these thermograms, various kinetic parameters, such as order of the degradation, energy of activation, frequency factor and entropy change have also been evaluated using Anderson-Freeman equation [34]:

$$\Delta \ln (dw/dt) = n(\Delta \ln W) - [(E/R)\, \Delta(1/T)] \quad (1)$$

where dw/dt is the rate of decomposition, W is the active mass, R is gas constant and T is temperature. n is order of degradation and E is energy of activation.

The frequency factor (A) and the entropy change (ΔS) were determined by following equations [35]:

$$A = (E\beta/RT^2)\, e^{E/RT} \quad (2)$$

$$\Delta S = R \ln (Ah/kT) \quad (3)$$

where β is heating rate (10°C per minute), h is Planck's constant and k is Boltzmann constant.

All the evaluated kinetic parameters are listed in Table 2 for all the compounds.

Table 2. The kinetic parameters of synthesized compounds derivatives.

Comp. code	*n*	*E* (kJ.mol^{-1})	*A* (s^{-1})	Δ*S* (J.mol^{-1}.K^{-1})
SNO series				
SNO-1 1st step **SNO-1 2nd step**	1.66 2.68	339.64 20.22	3.46 x 10^{17} 0.1473	234.18 -117.51
SNO -2	1.78	130.41	4.55 x 10^{7}	46.72
SNO -31st step **SNO-3 2nd step**	7.42 9.31	296.06 26.89	1.11 x 10^{21} 2.68	303.86 -90.88
SNO -4	8.55	171.10	5.48 x 10^{11}	125.67
SNO -5	10.80	209.76	6.34 x 10^{14}	184.39
SNO -6	9.34	2.11	0.0043	-143.46
SNO -7	3.64	50.56	734.03	-43.42
SNO -8	4.09	150.09	1.24 x 10^{11}	113.97
SNO -9	1.75	265.37	2.73 x 10^{21}	312.33
SNO -10	4.06	305.05	2.32 x 10^{24}	368.29
SNS Series				
SNS-1	2.65	392.51	8.33 x 10^{34}	571.16
SNS-2	0.22	598.65	3.05 x 10^{56}	984.42
SNS-3	2.84	16.03	9.60 x 10^{-01}	-97.25
SNS-4	7.73	620.61	5.25 x 10^{68}	1219.97
SNS-5	0.21	681.77	1.95 x 10^{82}	1480.47
SNS-6	0.27	564.66	1.72 x 10^{58}	1018.86
SNS-7	5.87	28.78	2.50 x 10^{01}	-70.24
SNS-8	2.28	7.78	1.09 x 10^{-01}	-114.55
SNS-9	1.58	29.58	1.25 x 10^{02}	-55.54
SNS-10	7.54	8.12	3.96 x 10^{-02}	-125.60

(Continued)

Table 2. The kinetic parameters of synthesized compounds derivatives.

Comp. code	*n*	*E* (kJ.mol^{-1})	*A* (s^{-1})	Δ*S* (J.mol^{-1}.K^{-1})
SSN Series				
SSN -1 1st step	1.98	97.42	3.4511 x 10^{3}	-34.50
SSN -1 2nd step	1.96	58.72	24.38	-76.68
SSN -2	2.90	25.94	1.83	-94.26
SSN -3	2.68	82.47	9.04 x 10^{4}	-4.18
SSN -4	2.02	49.36	2.14 x 10^{2}	-54.41
SSN -5	4.08	14.89	0.20	-112.00
SSN -6 1st step	1.19	98.67	3.36 x 10^{6}	26.19
SSN -6 2nd step	15.31	37.49	30.38	-70.36
SSN -6 3rd step	4.09	3.30	0.0069	-95.61
SSN -7	2	34.03	11.32	-78.87
SSN -8	1.95	64.08	1.47 x 10^{4}	-18.33
SSN -9	6.95	18.99	0.0056	-139.77
SSN -10	7.75	46.46	6.61 x 10^{2}	-43.73
SDN Series				
SDN-1 1st step	0.269	31.59	2.02 x 10^{13}	17.89
SDN-1 2nd step	0.429	58.20	1.17 x 10^{08}	-90.62
SDN-1 3rd step	0.314	38.25	1.24 x 10^{02}	-208.15
SDN-2 1st step	1.195	129.70	9.11 x 10^{52}	776.12
SDN-2 2nd step	0.211	68.17	8.27 x 10^{10}	-35.40
SDN-2 3rd step	1.531	272.69	3.44 x 10^{34}	43.92
SDN-2 4th step	0.655	103.09	8.61 x 10^{05}	-137.81
SDN-3 1st step	0.741	71.50	1.06 x 10^{12}	-13.86
SDN-3 2nd step	2.761	389.09	1.76 x 10^{51}	733.99
SDN-3 3rd step	0.539	134.68	4.74 x 10^{09}	-65.43
SDN-4 1st step	0.116	74.82	2.59 x 10^{08}	-85.75
SDN-4 2nd step	0.442	129.20	1.57 x 10^{08}	-94.47

(Continued)

Table 2. The kinetic parameters of synthesized compounds derivatives.

Comp. code	*n*	*E* (kJ.mol^{-1})	*A* (s^{-1})	Δ*S* (J.mol^{-1}.K^{-1})
SDO Series				
SDO-1 1st step	0.549	69.84	4.20×10^{23}	213.23
SDO-1 2nd step	0.435	129.70	2.05×10^{19}	129.13
SDO-2 1st step	0.506	53.21	2.30×10^{17}	93.25
SDO-2 2nd step	0.737	144.66	7.02×10^{23}	211.6
SDO-3 1st step	0.738	36.58	2.21×10^{10}	-41.72
SDO-3 2nd step	0.655	69.34	2.45×10^{11}	-26.28
SDO-4 1st step	0.661	33.26	4.11×10^{10}	-35.63
SDO-4 2nd step	0.591	41.57	1.61×10^{05}	-145.28
SDO-5 1st step	0.499	76.48	7.00×10^{24}	236.20
SDO-5 2nd step	0.302	89.79	1.70×10^{13}	7.960
SDO-5 3rd step	1.195	239.44	5.40×10^{22}	185.80

It is evident from table 2 that order of reactions is quite different in different compounds and in different steps. There is wide range of values of energy of activation (*E*), frequency factor (*A*) and entropy change (Δ*S*) for studied compounds.

SNO series.

Table 2 shows that the order of reactions is quite different in different steps for different dihydropyrimidinones. The order of reaction varies from 1.75 to 10.80 for single step degradation. For multistep degradation, it varies from 2.68 to 9.31. For single step degradation compounds, energy of activation is maximum for SNO-10 and minimum for SNO-6. The frequency factor also varies in the same order. For multi-step degradation compounds, in the first step, energy of activation is maximum for SNO-1 whereas in second step, it is maximum for SNO-3. The frequency factor is maximum for SNO-3 in first step and minimum for SNO-1 in second step.

Further, change in entropy (Δ*S*) for all the compounds is both positive and negative. The negative Δ*S* values indicate more ordered or more rigid structure whereas positive Δ*S* values indicate that the transition state is in less ordered state [36]. The highest value of entropy is for SNO-6 which has lowest energy of activation and frequency factor. The same but opposite order is for SNO-10 for single step degradation.

SSN series.

For single step decomposition, order of reaction varies from 1.95 to 7.75. For SSN-1, the order of reaction is almost same for both steps, difference is only of 0.02. However, much change is observed for different steps in SSN-6.

For single step degradation, energy of activation (E) is maximum for SSN-3 and minimum for SSN-5. The values of frequency factor (A) are quite different in first step. The frequency factor is maximum for SSN-3 and minimum for SSN-9. For multi-step degradation, in both SSN-1 and SSN-6, energy of activation and frequency factor is higher for the first step.

The entropy change is negative for all compounds except SSN-6 for the first step. The negative entropy indicates that the activation compound has a more ordered or more rigid structure than the reactants and reaction is slower than the normal whereas positive entropy indicates that the transition state is in less ordered state.

SNS series.

The order of reaction (n) varies from 0.21 to 7.54. The value of n is minimum for SNS-2 and maximum for SNS-4. The energy of activation (E) is highest for SNS-5 containing chloro group at 3rd position and minimum for SNS-8 which is without any substitution. The frequency factor (A) is also highest for SNS-5 but minimum for SNS-10. The entropy change is found to be both positive and negative.

SDN series.

The order of reaction is different in different steps for different compounds. For some compounds, it is less than one for most of the steps. The maximum order of reaction is found to be 2.761. However, for all the compounds, it is less than one for all the steps except 3rd step of SDN -5. The energy of activation (E) is highest for SDN-3 in second step while it is minimum in first step of SDN-1.

SDO series

In SDO series, the energy of activation is highest in third step of SDO-5 while lowest in first step of SDO-4. The frequency factor is highest for first step of SDO-2 and lowest for third step of SDO-1 compound. In SDO series, it is found to be maximum in first step of SDO-5 and minimum in second step of SDO-4 compound.

The entropy change is quite different for different compounds and the values are both positive and negative for different compounds. The positive values indicate that the transition state is less ordered than the original compound whereas negative entropy corresponds to an increase in the order of transition state than that of individual molecules.

From DSC, melting points of all the compounds are determined and are given in Table 3 along with melting points determined by open capillary method. There is good agreement between the values evaluated from DSC and those determined by open capillary method.

Comparison of thermal data of different series shows that if in one series a particular substitution increases the thermal stability, in the other series, it decreases.

Table 3. The melting temperatures (°C) of synthesized compounds by DSC and open capillary methods.

Compound code	DSC (°C)	Open capillary (°C)
SNO series		
SNO-1	168.81	168
SNO -2	153.72	152
SNO -3	181.01	179
SNO -4	181.55	182
SNO -5	162.84	164
SNO -6	158.84	160
SNO -7	170.27	171
SNO -8	199.11	198
SNO -9	168.83	169
SNO -10	144.15	145
SNS series		
SNS -1	138.89	140
SNS-2	119.32	118
SNS-3	190.57	190
SNS-4	167.13	168
SNS-5	156.85	157
SNS-6	130.87	130
SNS-7	98.68	101
SNS-8	89.82	90
SNS-9	79.86	81
SNS-10	162.17	164

(Continued)

Table 3. The melting temperatures (°C) of synthesized compounds by DSC and open capillary methods.

Compound code	DSC (°C)	Open capillary (°C)
SSN series		
SSN -1	179.20	180
SSN -2	193.62	194
SSN -3	210.31	211
SSN -4	253.14	254
SSN -5	192.87	194
SSN -6	167.74	167
SSN -7	233.34	235
SSN -8	246.60	247
SSN -9	237.12	238
SSN -10	206.81	208
SDN series		
SDN-1	122.74	123
SDN-2	153.91	153
SDN-3	191.76	193
SDN-4	201.55	202
SDN-5	212.95	214
SDO series		
SDO-1	158.05	160
SDO-2	294.60	294
SDO-3	292.18	292
SDO-4	249.24	250
SDO-5	147.27	148

Conclusions

It is concluded that thermal stability depends on structure of compound as well as substitutions. The position of substitution in aromatic ring skeleton also affects thermal stability and kinetic parameters. The kinetic parameters differ greatly for different compounds. No correlation could be established between kinetic parameters, melting temperature, thermal stability and substitution groups.

Disclosure statement

No potential conflict of interest was reported by the authors.

References

1. R.N. Mcelhaney, The use of differential scanning calorimetry and differential thermal analysis in studies of model and biological membranes, *Chem. Phys. Lipids*, **30**, 229-259 (1982).

2. P.L. Privalov, A.I. Dragan, Microcalorimetry of biological macromolecules, *Biophys. Chem.*, **126**, 16-24 (2007).

3. J. González-Rivera, C. Duce, D. Falconieri, C. Ferrari, L. Ghezzi, A. Piras, M.R. Tine, Coaxial microwave assisted hydrodistillation of essential oils from five different herbs (lavender, rosemary, sage, fennel seeds and clove buds): Chemical composition and thermal analysis, *Innov. Food Sci. Emerg. Technol.*, **33**, 308-318 (2016).

4. S.Z.D. Cheng, C.Y. Li, B.H. Calhoun, L. Zhu, W.W. Zhou, Thermal analysis: the next two decades, *Thermochim. Acta*, **355**, 59-68 (2000).

5. F.T. Martins, F.F. Guimarães, S.B. Honorato, A.P. Ayala, J. Ellena, Vibrational and thermal analyses of multicomponent crystal forms of the anti-HIV drugs lamivudine and zalcitabine, *J. Pharm. Biomed. Anal.*, **110**, 76-82 (2015).

6. M. Badea, R. Olar, L. Silvestro, M. Maurer, V. Uivarosi, Synthesis, spectral and thermal studies of the sodium salts of some Ru(III) complexes with quinolone antibiotics, *J. Thermal Anal. Calorim.*, **127**, 721-729 (2017).

7. R.K. Sharma, P. Ganesan, V.V. Tyagi, Long-term thermal and chemical reliability study of different organic phase change materials for thermal energy storage applications, *J. Thermal Anal. Calorim.*, **124**, 1357-1366 (2016).

8. L. André, S. Abanade , G. Flamant, Screening of thermo chemical systems based on solid-gas reversible reactions for high temperature solar thermal energy storage, *Renew. Sustain. Energy Rev.*, **64**, 703-715 (2016).

9. S. Wilczyński, The use of dynamic thermal analysis to distinguish between genuine and counterfeit drugs, *Int. J. Pharm.*, **490**, 16-21 (2015).

10. B.D.L. Ferreira, B.C.R. Araujo, R.C.O. Sebastião, M.I. Yoshida, W.N. Mussel, S.L. Fialho, J. Barbosa, Kinetic study of anti-HIV drugs by thermal decomposition analysis, *J. Thermal Anal. Calorim*., **127**, 577-585 (2017).

11. A.K. Attia, M.M. Ibrahim, M. Abdel-Nabi El-ries, Thermal analysis of some antidiabetic pharmaceutical compounds, *Adv. Pharm. Bull.*, **3**, 419-424 (2013).

12. S. Farah, T. Tsach, A. Bentolila, A. Domb, Morphological, spectral and chromatography analysis and forensic comparison of PET fibers, *Talanta*, **123**, 54-62 (2014).

13. R. Kumar, V. Sharma, N. Verma, P.K. Diwan, V. Kumar, V. Kumar, Analysis of writing/printing paper via Thermogravimetric Analysis: application in forensic science, *Aust. J. Forensic Sci.*, **51**(1), 22-39 (2019).

14. G. Martelli, C. Folli, L. Visai, M. Daglia, D. Ferrari, Thermal stability improvement of blue colorant C-Phycocyanin from *Spirulina platensis* for food industry applications, *Process Biochemistry*, **49**, 154-159 (2014).

15. J. González-Rivera, C. Duce, D. Falconieri, C. Ferrari, L. Ghezzi, A. Piras, M.R. Tine, Coaxial microwave assisted hydrodistillation of essential oils from five different herbs (lavender, rosemary, sage, fennel seeds and clove buds): Chemical composition and thermal analysis, *Innov. Food Sci. Emerg. Technol.*, **33**, 308-318 (2016).

16. H.J. Seifert, J. Peng, H.L. Lukas, F. Aldinger, Phase equilibria and thermal analysis of Si–C–N ceramics, *J. Alloys Compds*, **320**, 251-261 (2001).

17. Y. Xu, B. Fan, B. Xue, X. Zhang, Z. Luo, Q. Shen, H. Ma, Formation of hetero junction networks in the photoelectrical glass, ceramics: A Thermal analysis, *J. Am. Ceramic Soc.*, **99**, 2639-2644 (2016).

18. V.K. Thakur, M.K. Thakur, P. Raghavan, M.R. Kessler, Progress in green polymer composites from lignin for multifunctional applications: A review, *ACS Sustainable Chem. Eng.*, **2**, 1072-1092 (2014).

19. T. Defize, J.M. Thomassin, M. Alexandre, B. Gilbert, R. Riva, C. Jérôme, Comprehensive study of the thermo-reversibility of Diels-Alder based PCL polymer networks, *Polymer*, **84**, 234-242 (2016).

20. A.N. Frone, S. Berlioz, J.F. Chailan, D.M. Panaitescu, Morphology and thermal properties of PLA–cellulose nanofibers composites, *Carbohydrate Polym.*, **91**, 377-384 (2013).

21. J.M. Hutchinson, The application of thermal analysis to the study of epoxy–clay nanocomposites, *J. Thermal Anal. Calorim.*, **125**, 617-628 (2016).

22. F.A.A. Nugroho, A.D. de Zerio-Mendaza, C. Lindqvist, T.J. Antosiewicz, C. Müller, C. Langhammer, Plasmonic nano spectroscopy for thermal analysis of organic semiconductor thin films, *Anal. Chem.*, **89**, 2575-2582 (2017).

23. S. Nakamura, T. Saotome, A. Nakazawa, M. Fukuda, Y. Kuroda, S. Kidokoro, Thermodynamics of the thermal denaturation of acid molten globule state of cytochrome *c* indicate a reversible high-temperature oligomerization process, *Biochemistry*, **56**(18), 2372-2378 (2017).

24. X. Huang, G. Rein, Smouldering combustion of peat in wildfires: Inverse modelling of the drying and the thermal and oxidative decomposition kinetics, *Comb. Flame*, **161**, 1633-1644 (2014).

25. C. Gai, Y. Zhang, W.T. Chen, P. Zhang, Y. Dong, Thermogravimetric and kinetic analysis of thermal decomposition characteristics of low-lipid microalgae, *Bioresour. Technol.*, **150**, 139-148 (2013).

26. J. Cai, W. Wu, R. Liu, An overview of distributed activation energy model and its application in the pyrolysis of lignocellulosic biomass, *Renew. Sustain. Energy Rev.*, **36**, 236-246 (2014).

27. L.D. Zhao, S.H. Lo, Y. Zhang, H. Sun, G. Tan, C. Uher, C. Wolverton, V.P. Dravid, M.G. Kanatzidis, Ultralow thermal conductivity and high thermoelectric figure of merit in SnSe crystals, *Nature*, **508**, 373-377 (2014).

28. A. Zielińska, P. Oleszczuk, The conversion of sewage sludge into biochar reduces polycyclic aromatic hydrocarbon content and ecotoxicity but increases trace metal content, *Biomass and Bioenergy*, 75, 235-244 (2015).

29. K. Pielichowska, K. Pielichowski, Phase change materials for thermal energy storage, *Progress Mat. Sci.*, 65, 67-123 (2014).

30. E.J. Martínez**,** M.V. Gil, J.G. Rosas, R. Moreno, R. Mateos, A. Morán, X. Gómez, Application of thermal analysis for evaluating the digestion of microwave pretreated sewage sludge, *J. Thermal Anal. Calorim.*, **127**, 1209-1219 (2017).

31. T. Mori, M. Ohue, Y. Takii, T. Hashizume, T. Kato, K. Kotake, T. Sato, T. Tango, Factors predicting the response to oral fluoropyrimidine drugs: A phase II trial on the individualization of postoperative adjuvant chemotherapy using oral fluorinated pyrimidines in stage III colorectal cancer treated by curative resection (ACT-01 Study), *Oncology Report*, **29**, 437-444 (2016).

32. T.P. Selvam, C.R. James, P.V. Dniandev, S.K. Valzita, A mini review of pyrimidine and fused pyrimidine marketed drugs, *Research in Pharmacy*, **2**, 1-9 (2012).

33. J.W. Lee, H.J. Kim, K. Heo, Therapeutic aptamers: Developmental potential as anticancer drugs, *BMB Rep.*, **48**, 234-237 (2015).

34. D.A. Anderson, E.S. Freeman, The kinetics of the thermal degradation of polystyrene and polyethylene, *J. Polym. Sci*., **54** 253-260 (1961).

35. V.M. Kagathara, P.H. Parsania, Thermal analysis of cured chloro epoxy resins and epoxy–acrylate–styrene copolymers, *Polym. Test.*, **21**, 659-663 (2002).

36. A.P. Mishra, V.K. Tiwari, R. Singhal, Synthesis, characterization, thermal decomposition and kinetic parameters of Ni(II) and Cu(II) teraphthalate-8Hq complexes, *Ind. J. Chem.*, **41**, 2092-2095 (2002).

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