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Note

Relationship between the heat and the ratio of heat and temperature of the exothermic decomposition reaction of polynitroaromatic compounds

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Abstract

A relationship is established, using the least-squares method, between the heat of decomposition and the heat of decomposition divided by the peak absolute temperature.

Keywords: DSC; Heat of decomposition

In a previous paper [1], the relationship between the heat of decomposition and heat of explosion of forty-seven polynitroaromatic compounds (PNAC) was studied. In order to obtain information about the correlation of heats of decomposition (Q_{dec}) and the peak temperatures (T_m) of the exothermic decomposition reactions in the DSC curves of the PNACs, the values of Q_{dec} and T_m tabulated in Ref. [1] or [2] (for original data see Table 1) are fitted to the equation $Q_{\text{dec}} = 73.87 + 558.9(Q_{\text{dec}}/T_m)$ by the linear least-squares method.

Fig. 1 shows a linear interdependence between the parameters Q_{dec} and Q_{dec}/T_m for the exothermic decomposition reactions of forty-seven PNACs, indicating that

$$Q_{\text{dec}} = \frac{73.87T_m}{(T_m - 558.9)}$$

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Table 1
Data for forty-seven PNACs determined by DSC

No.	Compound	T_m/K	$Q_{dec}/kJ\ mol^{-1}$
1	Tetryl	486.4	1546
2	1,3-Diamino-2,4,6-trinitrobenzene	609.7	1097
3	1,3,5-Trinitrobenzene	685.4	1119
4	Hexanitrostilbene	624.6	1490
5	Picric acid	578.3	1166
6	<i>m</i> -Dinitrobenzene	711.7	721
7	<i>p</i> -Dinitrobenzene	709.4	665
8	2,3,4,6-Tetranitroaniline	510.2	1390
9	2,3,4,5-Tetranitroaniline	503.7	1147
10	2,3,5-Trinitrotoluene	616.0	1256
11	1,3,5-Triamino-2,4,6-trinitrobenzene	613.7	897
12	2,3,6-Trinitrotoluene	610.2	1131
13	2,3,4-Trinitrotoluene	572.7	1074
14	2,4,6-Trinitrotoluene	594.7	1053
15	2,4,5-Trinitrotoluene	571.7	1112
16	3,4,5-Trinitrotoluene	594.7	1102
17	2,4-Dinitrotoluene	586.2	850
18	2,5-Dinitrotoluene	637.0	709
19	2,4-Dinitrotoluene	585.2	897
20	3,5-Dinitrotoluene	652.2	587
21	2,6-Dinitrophenol	582.2	834
22	2,3-Dinitrotoluene	631.2	709
23	2,4-Dinitroaniline	645.0	732
24	3,4-Dinitrotoluene	614.2	777
25	2,6-Dinitrotoluene	630.0	718
26	2,4,6-Trinitrofluorobenzene	601.0	1244
27	2,4,6-Trinitroresorcin dimethyl ether	546.4	1430
28	2,4-Dinitrobenzaldehyde	567.2	860
29	2,6-Dinitroaniline	659.2	819
30	2,4,6-Trinitroxylene	603.4	982
31	5-Bromo-4,6-dinitroresorcinol dimethyl ether	596.7	932
32	Dinitro- <i>s</i> -trichlorobenzene	682.4	1063
33	3,5-Dinitrobenzoic acid	632.7	986
34	2,4-Dinitrochlorobenzene	666.0	537
35	2,4,6-Trinitroresorcinol	623.7	1034
36	2,4-Dinitrodiphenylamine	643.7	613
37	Dipicryl sulfone	594.4	2239
38	3,3',5,5'-Tetramino-2,2',4,4',6,6'-hexanitrobiphenyl	547.0	1696
39	Dipicryl sulfide	600.0	2325
40	4,6,10,12,16,18,22,24-Octanitro-2,8,14,20-tetraoxapentacyclo(19,3,1,1 ^{3,7} ,1 ^{9,13} ,1 ^{15,19})octacosal(25),3,5,7(28),9,11,13(27),15,17,19(26),21,23-dodecaene	646.0	3054
41	<i>s</i> -Tri(2,4-dinitrophenyloxy)trinitrobenzene	585.2	3632
42	Dipicrylamino-trinitrobenzene	528.4	2305
43	Bis(2,4-dinitrophenyl) sulfone	622.4	1615
44	<i>s</i> -Tripicrylamino-trinitrobenzene	549.7	4418
45	<i>s</i> -Tri(2,4-dinitrophenylamino)trinitrobenzene	590.4	2623
46	2,4-Dinitroanisole	567.2	860
47	Tripicrylmelamine	601.4	3366

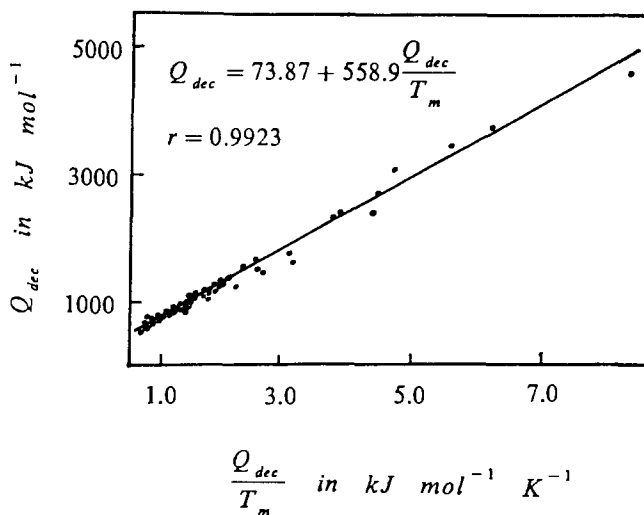


Fig. 1. The Q_{dec} vs. Q_{dec}/T_m relationship for the exothermic decomposition reaction of forty-seven PNACs.

References

- [1] Zhang Housheng, Hu Rongzu and Yang Desuo, Proc. Int. Symp. Pyrotech. Explos., China Academic Publishers, Beijing, 1987, p. 448.
- [2] Zhang Housheng, Hu Rongzu and Yang Desuo, Huaxue Tongbao, 12 (1987) 30.