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Analysis of differential scanning calorimetric data for reactive chemicals

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Abstract

In this report, the results of 849 differential scanning calorimetry (DSC) experiments for 820 reactive chemicals are presented. Exothermic onset temperatures (T_o) and heats of decomposition (Q) for those chemicals were analyzed to see if it is possible to classify their thermal hazards by these two factors. The values of the two factors, which were widely and uniformly distributed, were independent of each other based on statistical considerations. We report that it is possible to classify and to predict the thermal hazards of reactive chemicals by two-dimensional representation in terms of T_o and Q. The reactive chemicals were classified into 28 types according to the functional groups in the molecules. The proportion of exothermically decomposed samples and the mean values of T_o and Q for each type of compound were determined, and it has become apparent that the functional groups affect thermal stability. The effects of sample cell type (pinhole cell and sealed cell) and cell material on DSC results are also discussed.

Introduction

In recent years, the evaluation of chemical hazards has become important in the chemical industry because accidents such as explosions or fires tend to occur in batch processes where fine chemicals, including pharmaceuticals, and functional resins are produced. These accidents are mostly attributable to thermal hazards, such as runaway reactions or thermal decomposition of reactive chemicals, in the processes of synthesis, distillation or drying.

Differential scanning calorimetry (DSC) has been used widely for the evaluation of thermal hazards [1] in various industries as it is easy to operate, gives quantitative results, and gives information on sensitivity (exothermic onset temperature) and severity (heat of decomposition) at the same time. Differential scanning calorimetry, however, has intrinsic drawbacks caused by the very small quantity of sample used in the experiments. In particular, the exothermic onset temperatures obtained in DSC measurements cannot be applied directly to the determination of practical reaction temperatures or stor-

age temperatures, and the heats of decomposition have a relatively large error of 5–10% in each experiment.

In spite of these drawbacks, DSC is regarded as a useful tool for the evaluation of thermal hazards and for the investigation of decomposition mechanisms of reactive chemicals [2–5] if the experiments are carried out carefully.

In this report, the results of 849 DSC experiments for 820 chemicals having functional groups such as nitro or azo are presented [6,7] and analyzed to estimate the thermal hazards of the substances. The points at issue in the DSC measurements are also discussed.

2. Experimental

2.1 Materials

All chemicals used in this study were reagent grade and no further treatment was conducted.

2.2 Apparatus and procedures

A pressure DSC (DU Pont 910 pressure-type) was used for the measurement of thermal data of reactive chemicals. The experimental conditions are as follows:

(a) Heat rate: 10 K/min

(b) Sample mass: 1–2 mg

(c) Sample cell: An aluminum cell with a pin-hole (about 0.1 mm ϕ) on the lid (Fig. 1(a)) was used for all samples with the exception of some halogenated or volatile substances. For halogenated or volatile substances, a sealed stainless uncoated steel (SUS) cell (Fig. 1(b)) was used.

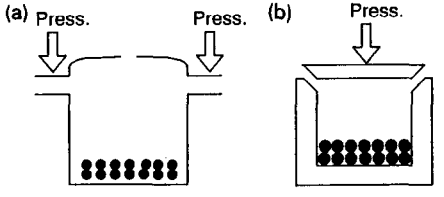

Fig. 1. Structures of sample cells: (a) aluminum pin-hole cell, and (b) sealed SUS cell.

(d) Atmosphere: Pressurized with argon to 3.5 MPa after flushing the environment three times with the gas when the pin-hole cell was used. The SUS cells were sealed in air under atmospheric pressure.

3. Results and discussion

3.1 Effect of sample cell material

It is well known that sample cell material may influence the decomposition of chemicals at relatively high temperatures. In particular, some halogenated compounds tend to react with an aluminum cell to produce aluminum halides at elevated temperatures, giving apparent exotherms on DSC curves.

Figure 2 shows DSC curves for 2,4,5-trichlorophenol (2,4,5-TCP) which was allowed to decompose in an aluminum pin-hole cell and a gold cell under an argon atmosphere. The compound reacts exothermically with aluminum at two temperature regions from about 270°C to 310°C and 400°C to 470°C. On the other hand, 2,4,5-trichlorobenzenesulfonyl chloride and methoxycarbonyl chloride do not show such apparent exotherms. Therefore, whether halogenated compounds react with aluminum or not may depend on the chemical structure of the compounds.

These DSC results demonstrate that it is preferable to use corrosion resistant cells, such as gold cells or gold-plated cells, for DSC measurements on halogenated compounds.

3.2 Effect of surrounding gas pressure or of sealing the cell

Some reactive chemicals do not show any exothermic decomposition due to evaporation or sublimation when heated at atmospheric pressure. Figure 3 shows DSC curves for 5-chloro-1,2,3-thiadiazole (5-CT) which was allowed to decompose in an aluminum pin-hole cell under nitrogen at different pressures.

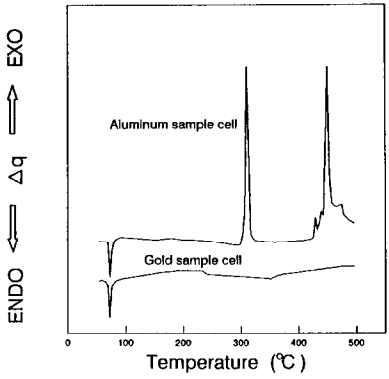

Fig. 2. Influence of sample cell material on the decomposition of 2,4,5-trichlorophenol.

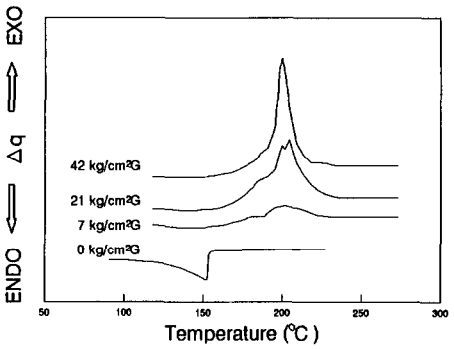

Fig. 3. Influence of nitrogen pressure on the decomposition of 5-chloro-1,2,3-thiadiazole in pinhole cell.

TABLE 1

Difference of DSC results (T_a and Q) between pressure type and sealed cell type for reactive chemicals

Chemical substances	Type	Exothermic onset temperature (T_a, °C)	Decomposition heat (Q, cal/g)
1 Benzoyl peroxide	Pressure	108	438
	sealed	113	369
2 *N*-Nitrosomethylurea	Pressure	66	316
	sealed	99	285
3 Acetaldoxime	Pressure	–	–
	sealed	–	–
4 Methoxycarbonyl chloride	Pressure	–	–
	sealed	–	–
5 Isoamyl nitrite	Pressure	159	137
	sealed	109	727
6 Azoxybenzene	Pressure	217	405
	sealed	241	329
7 Hydrazobenzene	Pressure	130	60
	sealed	179	40
8 Azobenzene	Pressure	308	191
	sealed	379	162
9 Pyridine-*N*-oxide	Pressure	251	380
	sealed	236	365
10 3,5-Dinitro-*o*-toluic acid	Pressure	266	444
	sealed	267	458
11 4-Methoxybenzyloxycarbonylazide	Pressure	106	289
	sealed	113	252
12 5-Diazouracil	Pressure	125	252
	sealed	114	271
13 2,3-Epoxy-1-propanol	Pressure	187	241
	sealed	115	441

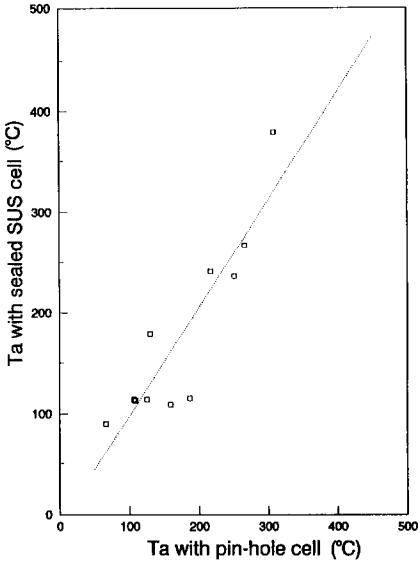

Fig. 4. Comparison of T_a with pin-hole cell and sealed cell type DSC for 11 substances.

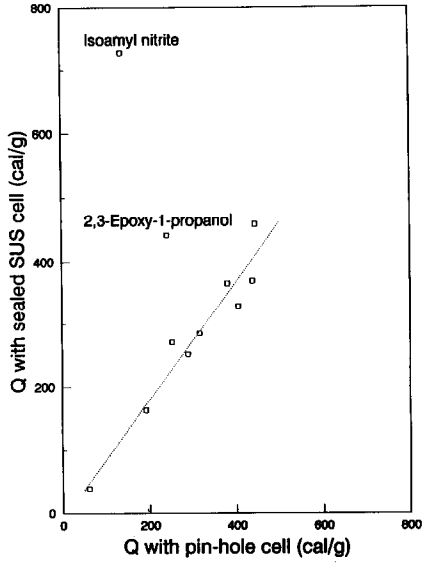

Fig. 5. Comparison of Q with pin-hole cell and sealed cell type DSC for 11 substances.

As the gas pressure in the cell increases, 5-CT tends to decompose more exothermically [8]. These exotherms are also observed when sealed cells are used. Measurements with sealed cells may be undesirable for investigations of re-

action kinetics, as secondary reactions will occur in the cell, but it is important to determine whether compounds so treated decompose exothermically.

On the other hand, there has been some opposition to the use of pin-hole cells, because a considerable amount of sample will evaporate or sublime from the pin-hole during heating. When the surrounding gas is highly pressurized, this amount is not large except for very volatile chemicals such as isoamyl nitrite. The decrease in sample weight from the pin-hole is easily confirmed by pressure thermogravimetry [9].

Differences between DSC data collected with the pin-hole cell and with the sealed cell are shown in Table 1 (13 substances), and the differences in adiabatic temperature, T_a or Q between the cells are shown in Figs. 4 and 5, respectively. The table and the figures show that the heats of decomposition and exothermic onset temperatures obtained by the two methods are similar except for isoamyl nitrite and 2,3-epoxy-1-propanol. The low heat of decomposition for isoamyl nitrite in a pin-hole cell is due to its evaporation from the pin-hole. The high heat of decomposition for 2,3-epoxy-1-propanol in a sealed cell may be due to residual air, which might initiate the thermal oxidation of the sample. Therefore, attention should be given to the type of sample cell and the atmosphere within it when reactive chemicals are allowed to decompose.

3.3 Baseline for thick SUS cells

When a thick SUS sealed cell is used to endure the high pressure generated in it, the DSC curve tends to become broad. For example, as is shown in Fig. 6, when the exothermic decomposition takes place immediately after melting, an endothermic peak of melting is sometimes not observed due to the time lag associated with the conduction of heat.

An apparent exotherm may also appear when a thick reference cell is used repetitively. This apparent exotherm is not negligible, yielding around 200 cal/g in the case of Fig. 7. This result may be attributed to the change in the heat capacity of the cell due to surface oxidation of the SUS cell.

For these reasons, it is preferable to use a thin sample cell for DSC experiments and, if thick sample cells like sealed SUS cell have to be used, the reference cell should not be used repeatedly.

3.4 Reproducibility of DSC experiments

Figure 8 shows the DSC results of lauroyl peroxide, performed to check the reproducibility of the measurements. As we have already described in the introduction of this report, the heat of decomposition (Q) shows a relatively large error of about 10%. As is shown in the figure, the reproducibility of the exothermic onset temperatures (T_0) is better than that of Q. Though DSC experiments were carried out only once for each reactive chemicals in this report, both T_0 and Q obtained seem to be valuable from the standpoint of the statistical analysis described below.

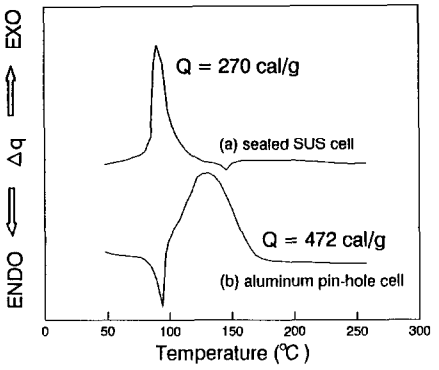

Fig. 6. Comparison of DSC curves of 2-chloroperbenzoic acid with SUS cell and aluminum cell.

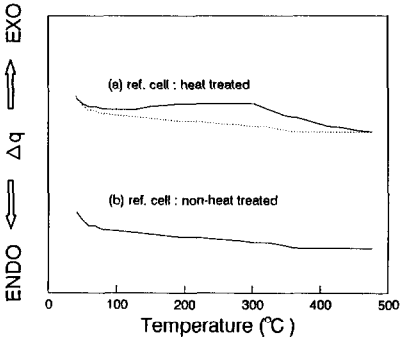

Fig. 7. Influence of heat treatment of reference cell (sealed SUS) on baseline of DSC.

3.5 Analysis of the collected data

3.5.1 Outline of the data

The thermal hazards of reactive chemicals must be evaluated from two aspects: the sensitivity, which shows how easily chemicals may decompose or ignite when a given amount of energy is supplied; and the severity, which shows how much or how fast energy is liberated when chemicals decompose.

The principle data obtained from an exothermic DSC curve are the exothermic onset temperatures T_a (the temperature at which the first deflection from the baseline is observed) and T_o (the temperature found by extrapolating the front baseline and the leading side of the peak to their intersection), and the heat of decomposition Q.

T_a and T_o, which can be a measure of the sensitivity of a substance, correlate well (correlation coefficient 0.966 (Fig. 9)) for 449 data points for which both T_o and T_a values are available. In this report, T_o was adopted as an index for sensitivity because it is easier to determine than T_a.

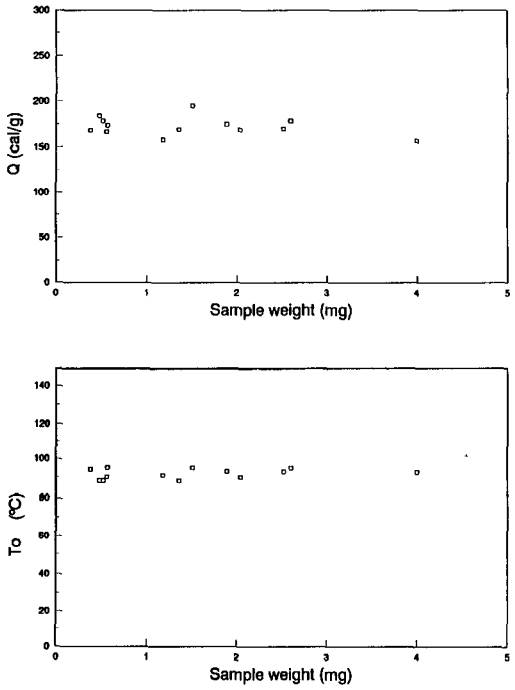

Fig. 8. Reproducibility of DSC results (T_o and Q) for lauroyl peroxide.

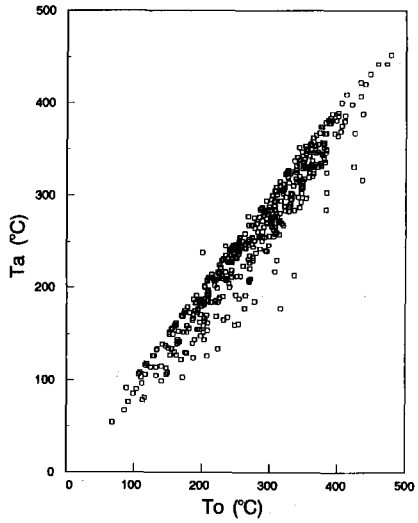

Fig. 9. Relation between exothermic onset temperatures T_o and T_a for 435 substances ($R=0.966$).

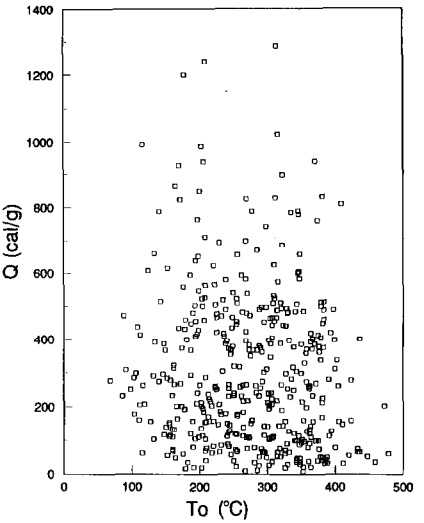

Fig. 10. Relation between exothermic onset temperature T_o and decomposition heat Q for 428 substances ($R=0.106$).

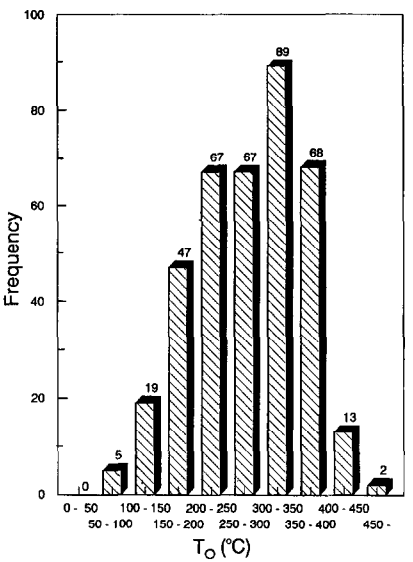

Fig. 11. Frequency distribution of T_o for 377 substances decomposed in aluminum pin-hole cell.

On the other hand, the correlation of exothermic onset temperature with heat of decomposition is low as shown in Fig. 10 (444 data points).

Figure 11 shows the frequency distribution for the exothermic onset temperatures (T_o) for 377 exothermically decomposed substances in the pin-hole cell, showing a uniform distribution over the temperature range of 150–400 °C.

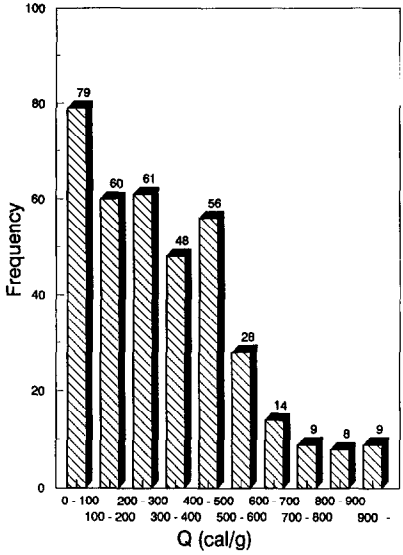

Fig. 12. Frequency distribution of Q for 377 substances decomposed in aluminum pin-hole cell.

A frequency distribution for the heats of decomposition of 372 compounds in the pin-hole cell is illustrated in Fig. 12. The figure shows that frequencies for heats of decomposition over 500 cal/g are extremely small, but the distribution of the values less than 500 cal/g is relatively uniform.

Therefore, the two parameters, exothermic onset temperature and heat of decomposition, may be appropriate factors to classify thermal hazards of reactive chemicals.

3.5.2 Thermal hazard evaluation with functional group

Thermally unstable chemicals such as peroxides or nitro compounds have specific functional groups, and initial stages of thermal decomposition processes will involve these groups when a certain amount of energy is applied. Therefore, there must be some relationship between the thermal hazards and the functional groups in the molecule.

In this report, 752 data points from 849 DSC experiments were obtained under the same experimental conditions with an aluminum pin-hole cell (the other 97 with the SUS cell) under argon at 3.5 MPa, and the compounds evaluated were classified into 28 types according to the functional groups defined in Table 2. In the table, substances containing more than two functional groups were listed in all the corresponding classifications. (Individual component data can be found in Tables 3 and 4 for the aluminum and SUS cell, respectively.)

Table 2 shows the proportion of samples decomposed exothermically and the mean values of exothermic onset temperatures (T_o) and heats of decomposition (Q) for each group. Over 98% of some reactive chemicals such as

TABLE 2

Means of T_0 and Q, and proportions of exothermically decomposed reactive chemicals in aluminum pin-hole cell

Functional groups	No. of samples	No. of exothermic samples	Proportions (%)	T_0 (°C)	Q (cal/g)
1 Organic peroxides	9	9	100	117	362
2 Nitroso compounds	15	13	87	194	230
3 Organic oximes	18	16	89	216	471
4 Acid chlorides	9	6	67	222	643
5 Nitrous esters	3	2	67	202	170
6 Azoxy compounds	3	3	100	293	445
7 Non-cyclic hydrazines	38	36	95	231	295
8 Azo compounds	15	15	100	243	237
9 *N*-oxides	9	9	100	284	285
10 Nitro compounds	115	113	98	300	506
11 Organic azides	2	1	50	-	289
12 Diazo compounds	0	0	-	-	-
13 Epoxy compounds	5	3	60	257	164
14 Alcohols	46	27	59	290	180
15 Phenols	68	41	60	266	257
16 Non-cyclic ethers	54	28	52	349	202
17 Aldehydes	34	17	50	305	256
18 Ketones	74	23	31	305	198
19 Carboxylic acid, esters	88	26	30	312	186
20 Non-cyclic amines	166	82	49	287	277
21 Non-cyclic amides	104	56	54	266	322
22 Cyano compounds	35	12	34	236	259
23 Non-cyclic organosulfides	112	71	63	258	220
24 Organophosphorus compounds	20	14	70	249	413
25 Organohalides	106	71	67	282	366
26 Heterocyclic compounds	61	13	21	302	266
27 Hydrocarbons	16	0	0	-	-
28 Others	4	2	50	252	486
Total number of data points	752	386	51.3		

organic peroxides, azo-compounds, *N*-oxides and nitro compounds decompose exothermically, while only 30–34% of ketones, carboxylic acids or cyano compounds do so. The overall proportion of samples which decomposed exothermically is 51.3%.

While peroxy compounds start to decompose at the relatively low temperature of 117°C, non-cyclic ethers, carboxylic acids, aldehydes, ketones, heterocyclic compounds and nitro compounds start to decompose at higher temperatures around 300–349°C. The heats of decomposition tend to decrease in the order of acid chlorides (643 cal/g), nitro compounds (506 cal/g), organic ox-

TABLE 3

Thermal data for some chemicals as obtained with the aluminum pin-hole cell

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min^2 g)
1	Abietic acid	1.10 Ar	3.5				
2	Acetaldoxime	1.51 Ar	3.5				
3	Acetamide	1.65 Ar	3.5	326.0			
4	Acetanilide	1.91 Ar	3.5				
5	Acetoacetanilide	1.08 Ar	3.5				
6	*o*-Acetoacetotoluidide	1.56 Ar	3.5				
7	Acetoaldehyde-ammonia	1.25 Ar	3.5				
8	4-Acetoamidoacetophenone	1.35 Ar	3.5				
9	*o*-Acetoanisidide	1.61 Ar	3.5	388.0	391.0	113.0	8.9
10	Acetohydroxamic acid	1.60 Ar	3.5	103.0	171.0	824.0	359.0
11	Acetone dicarboxylic acid	1.90 Ar	3.5				
12	Acetone semicarbazone	2.15 Ar	3.5				
13	Acetophenetidine	1.21 Ar	3.5				
14	Acetophenone	1.48 Ar	3.5				
15	*p*-Acetotoluide	1.89 Ar	3.5				
16	Acetoxime	1.33 Ar	3.5				
17	8-Acetoxyquinoline	1.92 Ar	3.5				
18	9-Acetylanthracene	1.80 Ar	3.5				
19	3-Acetyl-2,4-dimethylpyrrole	1.82 Ar	3.5				
20	3-Acetylindole	1.95 Ar	3.5				
21	Acetylsalicylic acid	1.31 Ar	3.5				
22	Adenine	1.55 Ar	3.5				
23	Adipoyl dihydrazide	1.12 Ar	3.5	256.4	282.9	262.6	5.7
24	Alizarin	1.45 Ar	3.5				
25	Allantoin	1.34 Ar	3.5	241.0	241.0	88.8	571.0
26	Allyl acetate	1.00 Ar	3.5				
27	Allyl amine	1.14 Ar	3.5				
28	2-Allyl-6-methylphenol	1.20 Ar	3.5				
29	2-Allyloxyethanol	1.30 Ar	3.5				
30	*o*-Allylphenol	1.86 Ar	3.5				
31	*m*-Aminoacetanilide	1.68 Ar	3.5				
32	*p*-Aminoacetophenone	1.22 Ar	3.5				
33	2-Aminoanthraquinone	1.90 Ar	3.5				
34	2-Aminobenzimidazole	1.15 Ar	3.5				
35	*p*-Aminobenzoyl hydrazide	1.86 Ar	3.5	280.0	295.0	115.0	3.9
36	2-Amino-3-chloro-1,4-naphthoquinone	1.25 Ar	3.5	315.0	343.0	99.5	115.0
37	2-Amino-4-chlorophenol	1.51 Ar	3.5	144.0	164.0	48.4	4.7
38	3-Amino-2-chloropyridine	1.40 Ar	3.5	309.0	314.0	489.0	∞
39	5-Amino-2-chloropyridine	1.12 Ar	3.5	302.0	319.0	389.0	∞
40	2-Amino-3,5-dibromopyridine	1.75 Ar	3.5	314.0	339.0	378.0	∞
41	4′-Amino-2′,5′-diethylbenzanilide	1.21 Ar	3.5	326.0	326.0	19.5	2.4
41	2-Amino-4,6-dihydroxypyrimidine	1.40 Ar	3.5				
43	4-Amino-2′,3-dimethylazobenzene	1.36 Ar	3.5	280.0	303.0	107.0	5.3
44	4-Amino-2,6-dimethylpyrimidine	1.77 Ar	3.5				
45	6-Amino-1,3-dimethyluracil	1.69 Ar	3.5				
46	2-Amino-6-ethoxybenzothiazole	1.30 Ar	3.5				

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min^2 g)
47	2-(2-Aminoethoxy)ethanol	1.32 Ar	3.5				
48	Aminoguanidine bicarbonate	1.06 Ar	3.5	252.0	255.0	67.0	10.5
49	4-Amino-3-hydrazino-5-mercapto-1,2,4-triazole	1.71 Ar	3.5	209.0	228.0	207.0	∞
50	2-Amino-5-mercapto-1,3,4-thiadiazole	1.52 Ar	3.5	244.0	244.0	146.0	∞
51	Aminomethanesulfonic acid	1.45 Ar	3.5				
52	2-Amino-5-methylbenzene-1-sulfonic acid	1.67 Ar	3.5	324.0	324.0		∞
53	4-Amino-2-methylbenzene-1-sulfonic acid	1.88 Ar	3.5				
54	4-Amino-3methylbenzene-1-sulfonic acid	1.84 Ar	3.5	336.0	336.0		∞
55	*trans*-4-Aminomethyl-1-cylcohexanecarboxylic acid	1.40 Ar	3.5				
56	3-Amino-5-methylisoxazole	1.40 Ar	3.5	188.0	254.0	446.0	∞
57	2-Amino-2-methyl-1-propanol	1.93 Ar	3.5				
58	3-(Aminomethyl)pyridine	1.22 Ar	3.5				
59	4-(Aminomethyl)pyridine	1.23 Ar	3.5				
60	2-Amino-5-methyl-1,3,4-thiadiazole	1.07 Ar	3.5	228.5	229.0	66.1	∞
61	4-Aminomorpholine	1.30 Ar	3.5				
62	2-Aminonicotinic acid	1.52 Ar	3.5				
63	2-Amino-4-nitroanisole	1.55 Ar	3.5	260.0	309.0	533.0	93.0
64	2-Amino-4-nitrophenol	1.48 Ar	3.5	152.0	173.0	201.0	25.0
65	2-Amino-5-nitrophenol	1.20 Ar	3.5	209.0	213.0	238.0	41.0
66	6-Amino-5-nitroso-2-thioruacil	1.43 Ar	3.5	209.0	271.0	218.0	∞
67	2-Amino-5-nitrothiazole	1.28 Ar	3.5	126.0	127.0	156.0	13.0
68	4-Amino-3-penten-2-one	1.37 Ar	3.5				
69	2-Amino-1-propene-1,1,3-tricarbonitrile	1.07 Ar	3.5	189.0	255.0	422.0	715.0
70	*N*-(3-Aminopropyl)morpholine	1.39 Ar	3.5				
71	3-Aminopyridine	1.64 Ar	3.5				
72	4-Aminopyridine	1.59 Ar	3.5				
73	4-Amino-2-thiopyrimidine	1.34 Ar	3.5				
74	4-Amino-1,2,4-traizole	1.51 Ar	3.5	178.0	263.0	483.0	31.7
75	*t*-Amylamine	1.12 Ar	3.5				
76	Amylbenzene	1.20 Ar	3.5				
77	n-Amylnitrile	2.62 Ar	4.9	183.0	202.0	203.0	30.0
78	Aniline	1.79 Ar	3.5				
79	3-Anilinopropionitrile	1.25 Ar	3.5				
80	Anthracene	1.41 Ar	3.5				
81	Anthraquinone	1.30 Ar	3.5				
82	Anthrone	1.61 Ar	3.5				
83	5-Azacytosine, hemihydrate	1.30 Ar	3.5				
84	8-Azaguanine	1.10 Ar	3.5	320.0	362.0	255.0	417.0
85	6-Azauracil	1.04 Ar	3.5	323.0	363.0	263.0	735.0
86	Azidotrimethylsilane	1.25 Ar	3.5				
87	Azobenzene	1.51 Ar	3.5	308.0	321.0	191.0	18.4
88	1,1′-Azobis(cyclohexane-1-carbonitrile)	1.54 Ar	3.5	118.0	118.0	208.0	213.0
89	2,2′-Azobisisobutyronitrile	1.85 Ar	3.5	106.0	106.0	299.0	∞
90	Azodicarbonamide	1.30 Ar	3.5	195.0	209.0	156.0	∞
91	4,4′-Azoxyanisole	1.85 Ar	3.5	256.0	305.0	347.0	194.0
92	Azoxybenzene	1.69 Ar	3.5	217.0	307.0	405.0	143.0
93	Benzalaniline	1.58 Ar	3.5				
94	Benzalazine	1.57 Ar	3.5	277.0	306.0	208.0	19.6
95	Benzaldehyde	1.83 Ar	3.5	255.0	255.0		11.0

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min^2 g)
96	Benzaldoxime	1.06 Ar	3.5	209.0	236.0	410.0	81.2
97	Benzal-*p*-toluidine	1.61 Ar	3.5				
98	Benzenesulfohydroxamic acid	1.47 Ar	3.5	96.0	111.0	205.0	31.2
99	Benzenesulfonamide	1.32 Ar	3.5	355.0	371.0	98.9	9.8
100	Benzenesulfonylhydrazide	1.40 Ar	3.5	113.0	147.0	387.0	91.0
101	Benzimidazole	1.40 Ar	3.5				
102	Benzonitrole	1.61 Ar	3.5				
103	Benzothiazole	1.85 Ar	3.5				
104	Benzotrifluoride	1.38 Ar	3.5	152.0	152.0	55.9	47.8
105	Benzoxazole	1.70 Ar	3.5				
106	2-Benzoxazolinone	1.32 Ar	3.5				
107	D,L-*N*-Benzoyl-α-alanine	1.83 Ar	3.5				
108	Benzoyl chloride	1.45 Ar	3.5	175.0	190.0	481.0	336.0
109	Benzoylhydrazine	1.32 Ar	3.5	223.0	260.0	259.0	7.1
110	Benzoyl peroxide	1.00 Ar	3.5	108.0	108.0	438.0	∞
111	3-Benzoylpropionic acid	1.33 Ar	3.5	305.0	307.0	38.6	3.2
112	3-Benzoylpyridine	1.54 Ar	3.5				
113	Benzoyltrifluoroacetone	1.62 Ar	3.5				
114	Benzylamine	1.58 Ar	3.5				
115	7-Benzylamino-4-nitrobenzoxadiazole	1.90 Ar	3.5	230.0	268.0	583.0	∞
116	*N*-Benzylbenzamide	1.51 Ar	3.5				
117	*S*-Benzyl-*N*-carbobenzyloxy-L-cysteine	1.74 Ar	3.5				
118	Benzyl chloride	1.84 Ar	3.5	169.0	172.0	269.0	∞
119	α-Benzyldioxime	1.48 Ar	3.5	227.0	238.0	387.0	233.0
120	Benzyl disulfide	1.21 Ar	3.5				
121	*N*-benzylethanolamine	1.82 Ar	3.5	350.0	353.0	21.9	4.7
122	Benzyl phenylacetate	1.43 Ar	3.5				
123	4-Benzylpiperidine	1.41 Ar	3.5				
124	4-Benzylpyridine	1.22 Ar	3.5				
125	Benzyl sulfide	1.11 Ar	3.5				
126	Benzylthiocyanate	1.62 Ar	3.5	236.0	254.0	117.0	17.7
127	Biacetylmonoxime	1.04 Ar	3.5	186.0	220.0	159.0	31.9
128	Bis(cyanoethyl)amine	1.58 Ar	3.5				
129	Bis(cyclohexanone)oxalyldihydrazine	1.10 Ar	3.5	227.0	270.0	219.0	134.0
130	1,8-Bis(*N,N*-dimethylamino)naphthalene	1.88 Ar	3.5	407.0	433.0	66.6	9.3
131	Bis(2,4-dinitrophenyl)oxalate	1.45 Ar	3.5	256.0	288.0	491.0	158.0
132	*N,N*-Bis(2-hydroxyethyl)-2-aminoethanesulfonic acid	1.67 Ar	3.5	285.0	307.0	107.0	30.5
133	Biuret	1.89 Ar	3.5	246.0	246.0	355.0	∞
134	2-Bromoacetoamide-4-nitrophenol	1.40 Ar	3.5				
135	9-Bromoanthracene	1.03 Ar	3.5				
136	4-Bromobenzenesulfonyl chloride	1.75 Ar	3.5				
137	3-Bromobenzonitrile	1.22 Ar	3.5				
138	4-Bromo-1-butene	1.38 Ar	3.5				
139	2-Bromo-n-butyric acid	1.53 Ar	3.5	76.0	91.0	309.0	68.2
140	α-Bromo-γ-butyrolactone	1.65 Ar	3.5	273.0	288.0	52.0	126.0
141	1-Bromo-4-chlorobutane	1.82 Ar	3.5				
142	1-Bromo-3-chloropropane	1.20 Ar	3.5				
143	2-Bromo-2-cyano-*N,N*-dimethylacetamide	1.43 Ar	3.5	173.0	193.0	105.0	27.2
144	5-Bromocytosine	1.06 Ar	3.5	251.0	259.0	318.0	∞

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min^2 g)
145	*N*-(2-Bromoethyl)phthalimide	1.87 Ar	3.5	329.0	354.0	97.0	87.6
146	1-Bromonaphthalene	1.32 Ar	3.5				
147	*p*-Bromophenacyl bromide	1.89 Ar	3.5	294.0	294.0	65.5	1.5
148	*β*-Bromophenetole	1.07 Ar	3.5	255.0	273.0	384.0	750.0
149	*p*-Bromophenylboric acid	1.08 Ar	3.5				
150	*β*-Bromostyrene	1.50 Ar	3.5	268.0	272.0	110.0	∞
151	2-Bromothiazole	1.43 Ar	3.5	165.0	232.0	471.0	321.0
152	2-Butene-1,4-diol	1.33 Ar	3.5				
153	2-Butoxynaphthalene	1.45 Ar	3.5				
154	n-Butylamine	1.46 Ar	3.5				
155	*t*-Butylamine	1.01 Ar	3.5				
156	Butylbenzene	1.89 Ar	3.5				
157	n-Butyl carbamate	1.82 Ar	3.5				
158	*t*-Butyl carbazate	1.63 Ar	3.5	240.0	240.0	150.0	33.5
159	4-*t*-Butylcyclohexanone	1.62 Ar	3.5				
160	*t*-Butyl-2-ethylperoxyhexanoate	1.38 N_2	0.1	69.0		213.8	
161	*t*-Butyl hydroperoxide	1.74 Ar	2.9	85.0	98.0	252.0	35.0
162	3-*t*-Butyl-4-hydroxy-5-methylphenylsulfide	1.46 Ar	3.5				
163	n-Butyl mercaptan	1.41 Ar	3.5				
164	*t*-Butyl perpivalate	2.61 Ar	3.5	54.0	68.0	277.0	49.0
165	4-*t*-Butylphenylthiophosphonic dichloride	1.48 Ar	3.5	155.0	196.0	417.0	19.4
166	tri-n-Butyl phosphate	1.27 Ar	3.5	310.4	314.3	54.1	00
167	n-Butyl phthalyl n-butyl glycolate	1.76 Ar	3.5				
168	*p*-*t*-Butylthiophenol	1.38 Ar	3.5				
169	*t*-Butyl-2,4,5-trichlorophenyl carbonate	1.41 Ar	3.5	236.0	246.0	369.0	153.0
170	Butylurea	1.53 Ar	3.5				
171	*ϵ*-Caprolactam	1.62 Ar	3.5	379.0	381.0	50.0	12.0
172	Carbanilide	1.04 Ar	3.5	312.0	319.0	51.8	5.5
173	Carbobenzyloxy-L-asparagine	1.42 Ar	3.5				
174	*N*-*ϵ*-Carbobenzyloxy-L-lysine	1.15 Ar	3.5				
175	Carbohydrazide	1.20 Ar	3.5	168.0	238.0	491.0	51.6
176	2-Carboxyethylphosphonic acid	1.79 Ar	3.5	177.0	194.0	410.0	47.5
177	3-Carboxypropyl disulfide	1.40 Ar	3.5				
178	L-(−)-Carvone	1.80 Ar	3.5				
179	2-Chloroacetamide	1.65 Ar	3.5	162.0	208.0	1241.0	696.0
180	4′-Chloroacetoacetanilide	1.00 Ar	3.5				
181	Chloroacetonitrile	1.51 Ar	3.5				
182	2′-Chloroacetophenone	1.42 Ar	3.5				
183	4-Chloroacetophenone	1.53 Ar	3.5				
184	*p*-Chloroanilidophosphoric acid	1.34 Ar	3.5	304.0	308.0	510.0	79.2
185	2-Chloroanthraquinone	1.48 Ar	3.5				
186	*p*-Chlorobenzaldehyde	1.35 Ar	3.5	281.0	314.0	219.0	12.7
187	*p*-Chlorobenzenesulfonic acid	1.43 Ar	3.5	103.0	110.0	161.0	16.0
188	*p*-Chlorobenzenesulfonyl chloride	1.26 Ar	3.5				
189	*p*-Chlorobenzoic acid	1.42 Ar	3.5	354.0	362.0	133.0	7.0
190	*o*-Chlorobenzoyl chloride	1.91 Ar	3.5	140.0	164.0	865.0	54.1
191	3-Chloro-2-butanone	1.85 Ar	3.5				
192	4-Chloro-6-(2,4-dihydroxyphenylazo)-1-hydroxybenzene-2-sulfonic acid	1.56 Ar	3.5	251.0	269.0	108.0	349.0

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min^2 g)
193	5-Chloro-2,4-dimethoxyaniline	1.39 Ar	3.5	246.0	268.0	397.0	454.0
194	1-Chloro-3,4-dinitrobenzene	2.15 Ar	3.5	345.0	367.0	403.0	65.0
195	2-Chloro-3,5-dinitrobenzoic acid	1.74 Ar	3.5	116.0	116.0	992.0	400.0
196	2-(2-Chloroethoxy)ethanol	1.47 Ar	3.5				
197	2-Chloro-6-fluorobenzaldehyde	1.12 Ar	3.5	302.0	330.0	254.0	28.0
198	4-Chloro-4'-fluorobutyrophenone	1.51 Ar	3.5				
199	2-Chloro-6-fluorotoluene	1.56 Ar	3.5				
200	2-Chloro-6-methoxypyridine	1.27 Ar	3.5				
201	3-Chloro-4-methylbenzonitrile	1.45 Ar	3.5				
202	4-Chloro-1-naphthol	1.36 Ar	3.5				
203	4-Chloro-2-nitroaniline	1.64 Ar	3.5	295.0	330.0	483.0	38.5
204	*p*-Chloronitrobenzene	1.19 Ar	3.5	324.0			
205	4-Chloro-3-nitrobenzoic acid	1.16 Ar	3.5	327.0	364.0	420.0	54.4
206	5-Chloro-2-nitrobenzotrifluoride	1.23 Ar	3.5	367.0	382.0	41.9	2.3
207	2-Chloro-5-nitropyridine	1.70 Ar	3.5	344.0	353.0	161.0	4.9
208	1-Chloro-2,3,4,5,6-pentabromocyclohexane	1.46 Ar	3.5				
209	5-Chloro-1-pentyne	1.48 Ar	3.5				
210	*m*-Chloroperbenzoic acid	1.73 Ar	3.5	91.0	88.0	472.0	41.4
211	2-Chlorophenothiazine	1.53 Ar	3.5				
212	3-Chloropropionitrile	1.78 Ar	3.5				
213	6-Chloropurine	1.52 Ar	3.5	173.0	182.0	34.5	∞
214	5-Chloro-3-pyridinol	1.07 Ar	3.5	306.0	320.0	494.0	∞
215	5-Chloro-1,2,3-thiadiazole	1.46 N_2	4.2	150.0		464.4	
216	1-Chloro-2-(trichloromethyl)benzene	1.27 Ar	3.4	180.0	200.0	850.0	406.0
217	2-Chloroxanthone	1.47 Ar	3.5	452.0	478.0	61.6	42.8
218	Cinnamic aldehyde	1.72 Ar	3.5	327.0	339.0	122.0	8.3
219	Cinnamonitrile	1.60 Ar	3.5				
220	*N*-Cinnamoyl-*N*-2,3-xylylhydroxylamine	1.64 Ar	3.5	152.0	177.0	193.0	10.5
221	Cinnamyl alcohol	1.83 Ar	3.5	323.0	330.0	28.9	1.2
222	Citraconic anhydride	1.27 Ar	3.5				
223	Citrazinic acid	1.61 Ar	3.5				
224	Copper(II) acetylacetonate	1.34 Ar	3.5				
225	Coumarin	1.40 Ar	3.5				
226	Cretainine	1.35 Ar	3.5				
227	Crotonic acid	1.65 Ar	3.5	349.2	360.9	37.8	3.5
227	Crotononitrile	1.54 Ar	3.5				
229	Cumene	1.95 Ar	3.5				
230	Cumene hydroperoxide	4.10 Ar	2.9	124.0	187.0	448.0	112.0
231	*o*-Cumenyl *N*-methylcarbamate	1.44 Ar	3.5				
232	Cyanoacetic acid	1.47 Ar	3.5	141.6	166.5	165.3	24.9
233	1-Cyanoacetylpiperidine	1.25 Ar	3.5	299.8	302.5	26.1	3.4
234	α-Cyano-4-hydroxy cinnamic acid	1.20 Ar	3.5				
235	2-Cyanopyridine	1.82 Ar	3.5				
236	3-Cyanopyridine	1.82 Ar	3.5				
237	4-Cyanopyridine	1.11 Ar	3.5				
238	Cyclohexanecarboxylic acid	1.38 Ar	3.5				
239	*trans*-1,2-Cyclohexanediamine-*N,N,N',N'*-tetraacetic acid	1.15 Ar	3.5				
240	1,3-Cyclohexanedione	1.42 Ar	3.5				

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min^2 g)
241	1,4-Cyclohexanedione	1.67 Ar	3.5				
242	1,2-Cyclohexanonedioxime	1.79 Ar	3.5	148.0	198.0	652.0	224.0
243	Cyclohexanoneoxime	1.80 Ar	3.5	126.0	207.0	527.0	17.2
244	Cyclohexene oxide	1.46 Ar	3.5				
245	Cyclohexylamine	1.56 Ar	3.5				
246	Cyclopentanone	1.43 Ar	3.5				
247	n-Decyl diphenyl phosphite	1.50 Ar	3.5	207.0	207.0		∞
248	Diacetamide	1.08 Ar	3.5				
249	1,2-Diacetoxyethane	1.54 Ar	3.5				
250	Diallylamine	1.44 Ar	3.5	314.3	314.3	52.2	6.5
251	1,2-Diamino-1,2-dicyanoethylene	1.56 Ar	3.5	187.0	187.0	294.0	∞
252	2,4-Diaminodiphenylamine	1.04 Ar	3.5				
253	4,4′-Diaminodiphenyl sulfide	1.67 Ar	3.5				
254	3,3-Diaminodiphenyl sulfone	1.13 Ar	3.5	422.0	433.0	75.1	30.1
255	4,4′-Diaminodiphenyl sulfone	1.87 Ar	3.5	324.0	339.0		99.7
256	*N,N′*-Diaminoguanidine HCl	1.57 Ar	3.5	187.0	194.0	456.0	45.7
257	2,4-Diamino-6-methyl-s-triazine	1.61 Ar	3.5				
258	1,4-Diazabicyclo-[2,2,2]-octane	1.51 Ar	3.5				
259	1,2-Dibenzanthracene	1.34 Ar	3.5				
260	2,2-Dibenzothiazyl disulfide	1.36 Ar	3.5				
261	5,5′-Dibromo-2,2′-dihydroxydiphenylsulfoxide	1.35 Ar	3.5	362.0	363.0		297.0
262	3,5-Dibromosalicylaldehyde	1.09 Ar	3.5				
263	*N,N*-Di-n-butylaniline	1.09 Ar	3.5				
264	3,5-Di-*t*-butyl-4-hydroxybenzoic acid	1.28 Ar	3.5				
265	Di-*t*-butylperoxide	2.44 N_2	4.3	127.0	162.0	133.0	12.0
266	3,5-Dichlorobenzonitrile	1.55 Ar	3.5				
267	2,6-Dichlorobenzoyl chloride	1.24 Ar	3.5	212.0	229.0	694.0	197.0
268	4,5-Dichloro-2-ethylaminoaniline	1.12 Ar	3.5	156.0	181.0	400.0	141.0
269	2,6-Dichloro-3-methylaniline	1.66 Ar	3.5				
270	2,6-Dichloro-4-nitroaniline	1.42 Ar	3.5	320.0	343.0	305.0	37.0
271	2,4-Dichlorophenol	1.58 Ar	3.5	259.0	262.0	232.0	109.0
282	2,4-Dichlorophenoxyacetic acid	1.56 Ar	3.5	352.0	379.0	501.0	∞
273	Dicyanodiamide	1.42 Ar	3.5	214.6	225.3	252.6	43.7
274	1,3-Dicyclohexylthiourea	1.70 Ar	3.5				
275	Diethylaminoacetone	1.36 Ar	3.5				
276	3-Diethylaminophenol	1.43 Ar	3.5				
277	4-Diethylaminosalicylic acid	1.00 Ar	3.5				
278	2,6-Difluorobenzamide	1.75 Ar	3.5	331.0	339.0	250.0	8.2
279	2,6-Difluorobenzonitrile	1.26 Ar	3.5				
280	1,2-Diformylhydrazine	1.81 Ar	3.5	234.0	234.0	304.0	380.0
281	9,10-Dihydroanthracene	1.54 Ar	3.5				
282	3,4-Dihydrocoumarin	1.27 Ar	3.5				
283	2,5-Dihydrofuran	1.21 Ar	3.5				
284	2′,4′-Dihydroxyacetophenone	1.82 Ar	3.5				
285	2′,5′-Dihydroxyacetophenone	1.73 Ar	3.5	337.0	344.0	47.3	2.5
286	3′,5′-Dihydroxyacetophenone	1.23 Ar	3.5	325.0	332.0	65.8	3.0
287	1,4-Dihydroxyanthracene	1.30 Ar	3.5				
288	2,4-Dihydroxybenzaldehyde	1.17 Ar	3.5				
289	4,6-Dihydroxy-2-mercaptopyrimidine	1.51 Ar	3.5	247.6	250.0	38.8	∞

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min² g)
290	3-(3,4-Dihydroxyphenyl)alanine	1.33 Ar	3.5				
291	2,5-Dimercapto-1,3,4-thiadiazole	1.35 Ar	3.5	207.8	207.8	69.4	18.1
292	2′-4′-Dimethoxyacetophenone	1.58 Ar	3.5				
293	3′,4′-Dimethoxyacetophenone	1.24 Ar	3.5				
294	3,4-Dimethoxy-1-allylbenzene	1.81 Ar	3.5	345.0	375.0	100.0	4.0
295	2,5-Dimethoxybenzaldehyde	1.85 Ar	3.5	362.0	362.0	121.0	3.9
296	2,4-Dimethoxybenzoic acid	1.26 Ar	3.5				
297	2,2-Dimethoxyethylamine	1.70 Ar	3.5				
298	3,4-Dimethoxyphenylacetone	1.13 Ar	3.5	375.0	405.0	157.0	7.6
299	(3,4-Dimethoxyphenyl)acetonitrile	1.22 Ar	3.5	386.0	410.0	149.0	11.8
300	*N,N*-Dimethylacetamide	1.36 Ar	3.5				
301	*p*(Dimethylamino)cinnamic aldehyde	1.32 Ar	3.5	331.0	350.0	94.3	15.2
302	3-(Dimethylamino)propionitrile	1.30 Ar	3.5				
303	*N,N*-dimethylaniline	1.52 Ar	3.5				
304	2,3-Dimethyl-2-butene	1.17 Ar	3.5				
305	*N,N*-Dimethylformamide	1.33 Ar	3.5				
306	Dimethylglyoxime	1.26 Ar	3.5	248.0	254.0	455.0	155.0
307	2,5-Dimethylhexane-2,5-dihydroperoxide	1.36 Ar	2.9	99.0	140.0	788.0	78.0
308	*O,O*-Dimethyl-*O*-(3-methyl-4-methylsulfinyl)phosphorothioate	1.25 Ar	3.5	153.0	165.0	202.0	11.5
309	*O,O*-Dimethyl-*O*-(3-methyl-4-nitrophenyl)phosphorothioate	1.66 Ar	3.5	169.0	221.0	624.0	242.0
310	*O,O*-Dimethyl-*O*-*p*-nitrophenylphosphorothioate	1.77 Ar	3.5	154.0	208.0	711.0	227.0
311	3,6-Dimethyl-4-octyne-3,6-diol	1.53 Ar	3.5	383.5	388.5	32.1	4.2
312	Dimethylolurea	1.00 Ar	3.5	191.6	263.4	113.9	47.6
313	Dimethylphenylphosphonite	1.74 Ar	3.5	330.0	423.0	160.0	∞
314	2,6-Dimethylpyridine	1.50 Ar	3.5				
315	2,6-Dimethyl-γ-pyrone	1.46 Ar	3.5	308.5	308.5	110.7	3.8
316	*N,N*-Dimetyl-*m*-toluidine	1.56 Ar	3.5				
317	*N,N*-Dimethyl-*p*-toluidine	1.62 Ar	3.5				
318	2,4-Dinitroaninline	3.09 N_2	4.9	302.0	346.0	779.0	220.0
319	2,6-Dinitroanaline	1.26 Ar	3.5	330.0	371.0	938.0	120.0
320	3,5-Dinitrobenzamide	2.39 Ar	3.5	335.0	381.0	833.0	140.0
321	2,4-Dinitrobenzoic acid	1.07 Ar	3.5	298.0	323.0	444.0	190.0
322	2,6-Dinitrobenzoic acid	1.01 Ar	3.5	231.0		250.0	
323	3,4-Dinitrobenzoic acid	1.17 Ar	3.5	293.0	345.0	790.0	220.0
324	3,5-Dinitrobenzoic acid	1.03 Ar	3.5	333.0	374.0	760.0	97.0
325	3,5-Dinitrobenzonitrile	1.69 Ar	3.5	380.0	409.0	810.0	140.0
326	3,4-Dinitrobenzylalcohol	2.13 Ar	3.5	206.0	269.0	826.0	150.0
327	3,5-Dinitrobenzylchloride	2.10 Ar	3.5	284.0	335.0	785.0	190.0
328	1,5-Dinitro-2,4-difluorobenzene	1.80 Ar	3.5	355.0	379.0	514.0	33.5
329	2,4-Dinitrodiphenylamine	1.66 Ar	3.5	308.0	348.0	658.0	77.0
330	2,4-Dinitro-1-naphthol	1.46 Ar	3.5	206.6	206.6	459.5	∞
331	2,4-Dinitrotoluene	1.84 Ar	3.5	271.0	312.0	829.0	170.0
332	3,4-Dinitrotoluene	2.00 Ar	3.5	284.0	322.0	898.0	350.0
333	3,5-Dinitro-*o*-toluic acid	1.06 Ar	3.5	266.0	307.0	444.0	189.0
334	1,5-Diphenylcarbazide	1.51 Ar	3.5	164.0	204.0	196.0	19.0
335	Diphenyl disulfide	1.44 Ar	3.5				

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min² g)
336	Diphenyl ether	1.49 Ar	3.5				
337	*N,N*-Diphenylformamide	1.40 Ar	3.5				
338	1,3-Diphenylguanidine	1.65 Ar	3.5				
339	Diphenyl phosphite	1.56 Ar	3.5				
340	1,1-Diphenyl-2-picrylhydrazine	1.44 Ar	3.5	170.0	170.0	926.0	89.6
341	1,1-Diphenyl-2-picrylhydrazyl	1.75 Ar	3.5	133.0	133.0	660.0	21.3
342	1,4-Diphenylsemicarbazide	1.44 Ar	3.5	208.0	220.0	83.8	2.0
343	4,4-Diphenylsemicarbazide	1.68 Ar	3.5				
344	*sym*-Diphenylthiourea	1.27 Ar	3.5				
345	5,5'-Dithiobis(2-nitrobenzoic acid)	1.45 Ar	3.5	249.0	255.0	510.0	129.0
346	2,2-Dithiobis(5-nitropyridine)	1.01 Ar	3.5	207.2	268.0	424.1	81.0
347	2,2'-Dithiosalicylic acid	1.15 Ar	3.5				
348	1,3-Di-*o*-tolylguanidine	1.38 Ar	3.5	191.0	191.0	20.4	4.2
349	*sym*-Di-*o*-tolylthiourea	1.69 Ar	3.5				
350	*sym*-Di-*p*-tolylthiourea	1.47 Ar	3.5				
351	1,2-Epoxybutane	1.92 Ar	3.5				
352	2,3-Epoxy-1-propanol	1.47 Ar	3.5	187.0	197.0	241.0	5.9
353	*N*-(2,3-Epoxypropyl)phthalimide	1.30 Ar	3.5	272.0	300.0	143.0	13.2
354	1,2-Ethanedithiol	1.70 Ar	3.5				
355	3-Ethoxy-2-cyclohexen-1-one	1.40 Ar	3.5				
356	3-Ethoxy-4-hydroxybenzaldehyde	1.28 Ar	3.5	338.0	351.0	103.0	4.5
357	2-Ethoxynaphthalene	1.56 Ar	3.5	341.8	357.8	274.7	∞
358	2-Ethylanthraquinone	1.44 Ar	3.5	430.8	447.3	53.1	18.7
359	Ethylbenzene	1.70 Ar	3.5				
360	Ethyl benzoate	1.20 Ar	3.5				
361	2-Ethylbutyraldehyde	1.36 Ar	3.5				
362	Ethyl carbazate	1.28 Ar	3.5	250.0	254.9	178.9	26.4
363	Ethyl 2-chloroacetoacetate	1.22 Ar	3.5	192.0	207.0	155.0	40.3
364	Ethyl diethylphosphonoacetate	1.44 Ar	3.5	347.0	347.0	88.0	∞
365	Ethylene glycol monobenzyl ether	1.44 Ar	3.5				
366	Ethylene thiourea	1.58 Ar	3.5				
367	Ethyl *N*-ethylcarbamate	1.43 Ar	3.5				
368	Ethyl formate	1.17 Ar	3.5				
369	Ethyl 2-furoate	1.81 Ar	3.5				
370	Ethyl gallate	1.58 Ar	3.5	335.0	348.0	29.0	14.5
371	2-Ethylimidazole	1.10 Ar	3.5				
372	*N*-Ethyle-*N*-methylaniline	1.75 Ar	3.5				
373	*N*-Ethylmorpholine	1.46 Ar	3.5				
374	Ethyl *N*-phenylcarbamate	1.76 Ar	3.5				
375	Ethyl-posphite	1.59 Ar	3.5	108.0	149.0	367.0	∞
376	3-Ethylrhodamine	1.49 Ar	3.5				
377	*N*-Ethyl-*p*-toluenesulfonamide	1.16 Ar	3.5				
378	Ethyl-*p*-toluenesulfonate	1.79 Ar	3.5	268.0	268.0		∞
379	*N*-Ethyl-*o*-toluidine	1.49 Ar	3.5				
380	Fluorene	1.46 Ar	3.5				
381	Fluoren-9-one	1.30 Ar	3.5				
382	*o*-Fluoroacetophenone	1.28 Ar	3.5				
383	3-Fluorobenzaldehyde	1.82 Ar	3.5	294.0	315.0	65.4	4.7
384	Fluorobenzene	1.43 Ar	3.5				
385	4-Fluoro-3-nitrophenylazide	1.62 Ar	3.5	129.0	177.0	1200.0	142.0

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min^2 g)
386	4-Fluoro-2-nitrotoluene	1.34 Ar	3.5	319.0	357.0	198.0	8.6
387	4-Fluorophenoxyacetic acid	1.23 Ar	3.5	340.0	340.0	99.2	14.0
388	Formanilide	1.13 Ar	3.5				
389	1-Formylpiperazine	1.33 Ar	3.5				
390	Fumaric acid	1.42 Ar	3.5	322.7	322.7	144.9	70.3
391	Fumaric acid monoethyl ester	1.20 Ar	3.5				
392	Fumaronitrile	1.39 Ar	3.5				
393	Furfuryl mercaptan	1.46 Ar	3.5	238.0	246.0	57.9	22.2
394	2-Furildioxime	1.50 Ar	3.5	187.8	225.3	467.6	∞
395	α-Furoic acid	1.27 Ar	3.5				
396	*N*-(γ-L-Glutamyl)phenylalanine	1.55 Ar	3.5				
397	Glutaric acid	1.33 Ar	3.5	212.8	335.8	282.9	12.5
398	Glycocyamine	1.41 Ar	3.5				
399	Glycylglycine	1.23 Ar	3.5				
400	1-Heptyne	1.43 Ar	3.5				
401	Hexamethylene tetramine	1.61 Ar	3.5	326.0	326.0	158.0	∞
402	2,5-Hexanedione	1.48 Ar	3.5				
403	3-Hexanone	1.11 Ar	3.5				
404	α-Hexylcinnamaldehyde	1.45 Ar	3.5				
405	2-Hexyloxyethanol	1.88 Ar	3.5				
406	Hippuric acid	1.46 Ar	3.5				
407	Hydantoic acid	1.52 Ar	3.5				
408	2-Hydrazinobenzothiazole	1.10 Ar	3.5	230.5	237.6	180.3	9.8
409	Hydrazobenzene	1.47 Ar	3.5	130.0	175.0	60.0	9.4
410	Hydroquinone	1.31 Ar	3.5				
411	*o*-Hydroxyacetophenone	1.28 Ar	3.5				
412	1-Hydroxybenzotriazole	2.21 Ar	3.5	167.0	204.0	501.0	281.0
413	2-Hydroxyethylhydrazine	1.01 Ar	3.5	242.0	251.0	240.	73.8
414	1-(2-Hydroxyethyl)-piperazine	1.12 Ar	3.5				
415	*N*-2-Hydroxyethylpiperazine-*N'*-3-propanesolfonic acid	1.61 Ar	3.5	284.1	292.6	66.2	12.6
416	5-Hydroxyindole-3-acetic acid	1.11 Ar	3.5				
417	L-3-Hydroxykynurenine	1.44 Ar	3.5				
418	3-Hydroxy-4-methoxycinnamic acid	1.46 Ar	3.5	378.0	388.0	50.4	3.9
419	*N*-(Hydroxymethyl)-acrylamide	1.53 Ar	3.5	137.4	146.0	296.4	284.0
420	3-Hydroxy-1-methylpiperidine	1.60 Ar	3.5				
421	1-Hydroxy-2-naphthoic acid	1.23 Ar	3.5				
422	2-Hydroxy-3-naphthoic acid	1.11 Ar	3.5				
423	2-Hydroxy-1,4-naphthoquinone	1.47 Ar	3.5	201.2	202.8	19.0	∞
424	2-Hydroxy-3-naphthoic acid hydrazide	1.93 Ar	3.5	210.0	209.6	77.8	4.5
425	8-Hydoxy-5-nitroquinoline	0.99 Ar	3.5	247.4	273.2	367.5	30.2
426	7-Hydroxy-3*H*-phenoxazin-3-one-10-oxide sodium salt	1.26 Ar	3.5	229.0	275.0	151.0	11.3
427	*p*-Hydroxyphenylpyruvic acid	1.33 Ar	3.5				
428	3-Hydroxypyridine	1.48 Ar	3.5	377.7	385.9	42.6	39.6
429	4-Hydroxypyridine	1.37 Ar	3.5	398.2	420.2	55.6	6.9
430	4-Hydroxy-2-quinolinecarboxylic acid n-hydrate	1.51 Ar	3.5				
431	Hydroxyurea	1.62 Ar	3.5	139.1	141.6	515.0	∞
432	Hypoxanthine	1.18 Ar	3.5				
433	Imidazole	1.84 Ar	3.5				
434	Iminodiacetic acid	1.45 Ar	3.5				
435	2,2'-Iminodiethanol	1.31 Ar	3.5	319.8	326.3	70.7	9.3

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min^2 g)
436	Isoamyl nitrite	1.48 Ar	3.5	159.0	202.0	137.0	15.5
437	Isonicotinaldehyde	1.39 Ar	3.5	244.9	253.6	22.5	35.1
438	Isonicotinaldoxime	1.86 Ar	3.5	204.0	239.0	580.0	308.0
439	Isonicotinic acid hydrazide	0.90 Ar	3.5	274.2	302.2	103.5	8.0
440	Isonitrosoacetophenone	1.25 Ar	3.5	127.0	153.0	615.0	149.0
441	Isophthalonitrile	1.32 Ar	3.5				
442	Isophthaloyl chloride	1.00 Ar	3.5				
443	Isophthaloyldihydrazide	1.58 Ar	3.5	240.0	293.0	275.0	26.1
444	Isopropanolamine	1.33 Ar	3.5				
445	*o*-Isopropoxyphenyl-*N*-methylcarbamate	1.70 Ar	3.5				
446	Isopropyl benzoate	1.77 Ar	3.5				
447	Isopropyl formate	1.01 Ar	3.5				
448	Isopropyl nitrite	4.36 Ar	4.9				
449	iso-Quinoline	1.88 Ar	3.5				
450	Lactamide	1.07 Ar	3.5	286.8	287.7	25.3	21.6
451	Lauroyl peroxide	3.67 Ar	3.5	67.0	86.0	232.0	27.0
452	Lauryl gallate	1.39 Ar	3.5				
453	2,4-Lutidine	1.64 Ar	3.5				
454	2,6-Lutidine-1-oxide	1.32 Ar	3.5	261.0	288.0	233.0	93.4
455	Maleic acid	1.62 Ar	3.5		302.2	204.5	16.9
456	Maleic anhydride	1.27 Ar	3.5	270.0	280.5	78.0	28.1
457	Malonamide	0.92 Ar	3.5				
458	Malonic acid	2.01 Ar	3.5				
458	Malonyldihydrazide	1.49 Ar	3.5	197.0	208.0	564.0	26.1
460	Mandelonitrile	1.38 Ar	3.5				
461	Melamine	1.28 Ar	3.5	381.1	384.7	32.7	∞
462	β-Mercaptopropionic acid	1.86 Ar	3.5				
463	6-Mercaptopurine monohydrate	1.29 Ar	3.5	328.8	347.8	47.3	3.7
464	Mesityl oxide	1.68 Ar	3.5				
465	Metanil yellow	1.24 Ar	3.5	319.0	326.0	62.3	111.0
466	Methacrylonitrile	1.36 Ar	3.5				
467	2-Methoxyacetophenone	1.38 Ar	3.5				
468	*p*-Methoxyazobenzene	1.82 Ar	3.5	349.0	367.0	157.0	95.0
469	4-Methoxybenzyloxycarbonylazide	1.03 Ar	3.5	106.0		289.0	
470	Methoxycarbonyl chloride	1.00 Ar	3.5				
471	Methoxycarbonyl chloride	~1 Ar	3.5				
472	2-Methoxyfuran	1.36 Ar	3.5	277.6	267.1	9.9	1.7
473	2-Methoxynaphthalene	1.61 Ar	3.5				
474	2-Methoxy-5-nitropyridine	1.43 Ar	3.5	313.6	347.8	584.0	∞
475	6-Methoxyquinoline	1.34 Ar	3.5				
476	4-Methoxy-α-toluenethiol	1.66 Ar	3.5	276.0	276.0		3.5
477	Methyl acetoacetate	1.78 Ar	3.5				
478	*N*-Methylaniline	1.22 Ar	3.5				
479	2-Methylanthraquinone	1.12 Ar	3.5	441.9	458.6	35.1	17.8
480	5-Methyl-1*H*-benzotriazole	1.77 Ar	3.5	313.3	327.5	298.0	24.6
481	Methyl carbamate	1.12 Ar	3.5				
482	Methyl cinnamate	1.71 Ar	3.5				
483	2-Methyl-1,3-cyclopentadione	1.39 Ar	3.5	287.8	298.6	49.4	82.0
484	2-Methyl-4,6-di-*t*-butylphenol	1.14 Ar	3.5				
485	Methyl-3,4-dichlorocarbanilate	1.82 Ar	3.5	381.0	397.0	491.0	819.0

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min^2 g)
486	Methyl-3,5-dimethoxybenzoate	1.37 Ar	3.5				
487	4-Methyl-1,3-dioxolan-2-one	1.72 Ar	3.5				
488	Methyl disulfide	1.54 Ar	3.5				
489	*N*-Methylformanilide	1.91 Ar	3.5				
490	*N*-Methylmorpholine	1.47 Ar	3.5				
491	*N*-Methyl-*N*-nitrosoaniline	1.48 Ar	3.5	171.0	198.0	429.0	31.0
492	2-Methyl-2-nitrosopropane, dimer	1.08 Ar	3.5	106.0	147.0	117.0	5.3
493	*N*-Methyl-*N*-nitroso-*p*-toluenesulfonamide	1.74 Ar	3.5	78.0	112.0	414.0	62.6
494	3-Methyl-1-pentyn-3-ol	1.78 Ar	3.5	353.2	352.6	7.5	6.1
495	1-Methyl-2-phenoxyethylamine	1.36 Ar	3.5				
496	2-Methylpyridine	1.11 Ar	3.5				
497	*N*-Methyl-2-pyridone	1.71 Ar	3.5				
498	*N*-Methyl-2-pyrrolidone	1.42 Ar	3.5				
499	Methyl red	1.03 Ar	3.5	188.0	205.0	186.0	668.0
500	1-Methyl-1,2,3,4-tetrazole-5-thiol	1.04 Ar	3.5	176.9	194.0	639.1	76.0
501	2-Methyl-1,3,4-thiadiazole-5-thiol	1.72 Ar	3.5	294.1	307.1	36.1	14.0
502	*p*-(Methylthio)benzoic acid	1.60 Ar	3.5	409.0	412.0	31.7	3.4
503	(Methylthio)methyl-*p*-tolylsulfone	1.52 Ar	3.5	242.0	242.0	122.0	528.0
504	4-Methyl-2-thiouracil	1.43 Ar	3.5				
505	Methyl *p*-toluenesulfonate	1.77 Ar	3.5	336.0	362.0	92.4	389.0
506	2-(*N*-Morpholino)ethanesulfonic acid, monohydrate	1.95 Ar	3.5	316.2	435.6	66.4	55.4
507	α-Naphthoquinoline	1.73 Ar	3.5				
508	α-Naphthoquinone	1.26 Ar	3.5	246.7	263.4	185.0	88.5
509	1-Naphtylamine-6-sulfonic acid	1.64 Ar	3.5				
510	Nicotinaldehyde	1.44 Ar	3.5				
511	Nicotinamide	1.28 Ar	3.5				
512	Nicotinic acid *N*-oxide	1.64 Ar	3.5	266.0	302.0	241.0	31.5
513	Nicotinohydrazide	1.42 Ar	3.5	251.3	276.8	159.9	9.1
514	*m*-Nitroacetoanilide	2.60 Ar	3.5	324.0	383.0	490.0	∞
515	*o*-Nitroacetonanilide	2.58 Ar	3.5	323.0	364.0	394.0	159.0
516	*p*-Nitroacetoanilide	2.62 Ar	3.5	303.0	383.0	514.0	∞
517	*m*-Nitroacetophenone	2.35 Ar	3.5	283.0	327.0	442.0	95.1
518	*o*-Nitroacetophenone	2.46 Ar	3.5	288.0	328.0	494.0	168.0
519	*p*-Nitroacetophenone	2.45 Ar	3.5	258.0	313.0	466.0	67.2
520	*m*-Nitroaniline	2.14 Ar	3.5	315.0	347.0	605.0	114.0
521	*o*-Nitroaniline	2.44 Ar	3.5	298.0	341.0	485.0	38.1
522	*p*-Nitroaniline	2.30 Ar	3.5	308.0	345.0	601.0	96.6
523	*m*-Nitroanisole	2.63 Ar	3.5	343.0	376.0	379.0	73.1
524	*o*-Nitroanisole	2.62 Ar	3.5	328.0	357.0	359.0	34.1
525	*p*-Nitroanisole	2.62 Ar	3.5	347.0	370.0	387.0	65.3
526	*m*-Nitrobenzaldehyde	2.44 Ar	3.5	243.0	262.0	594.0	∞
527	*o*-Nitrobenzaldehyde	2.22 Ar	3.5	216.0	223.0	506.0	141.0
528	*p*-Nitrobenzaldehyde	1.53 Ar	3.5	255.0	285.0	670.0	∞
529	*m*-Nitrobenzamide	2.63 Ar	3.5	346.0	382.0	450.0	56.3
530	*o*-Nitrobenzamide	2.45 Ar	3.5	330.0	358.0	371.0	38.0
531	*p*-Nitrobenzamide	2.44 Ar	3.5	349.0	383.0	462.0	56.9
532	*p*-Nitrobenzene	2.49 Ar	3.5	389.0	400.0	312.0	121.0
533	*p*-Nitrobenzeneazoresorcinol	1.34 Ar	3.5	144.0	203.0	524.0	96.3
534	*p*-Nitrobenzenorcinol	1.75 Ar	3.5	167.0	187.0	368.0	557.0
535	*p*-Nitrobenzenesulfonic acid	2.82 N_2	4.9	126.0	129.0		39.0

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min^2 g)
536	*m*-Nitrobenzhydrazide	2.21 Ar	3.5	199.0	222.0	567.0	19.2
537	*o*-Nitrobenzhydrazide	2.24 Ar	3.5	185.0	277.0	789.0	186.0
538	*p*-Nitrobenzhydrazide	2.23 Ar	3.5	224.0	225.0	478.0	14.5
539	5-Nitrobenzimidazole	1.62 Ar	3.5	317.1	350.2	299.1	35.9
540	*m*-Nitrobenzoic acid	2.61 Ar	3.5	331.0	375.0	414.0	99.9
541	*o*-Nitrobenzoic acid	2.37 Ar	3.5	263.0	305.0	387.0	38.1
542	*p*-Nitrobenzoic acid	2.60 Ar	3.5	338.0	379.0	406.0	149.0
543	*m*-Nitrobenzoic acid methyl ester	2.39 Ar	3.5	369.0	403.0	338.0	117.0
544	*o*-Nitrobenzoic acid methyl ester	2.48 Ar	3.5	344.0	377.0	362.0	48.5
545	*p*-Nitrobenzoic acid methyl ester	2.39 Ar	3.5	364.0	399.0	399.0	131.0
546	*p*-Nitrobenzonitrile	1.50 Ar	3.5				2.0
547	*p*-Nitrobenzoyl chloride	1.52 Ar	3.5	277.0	310.0	525.0	110.0
548	*m*-Nitrobenzyl alcohol	2.32 Ar	3.5	287.0	343.0	507.0	113.0
549	*o*-Nitrobenzyl alcohol	2.46 Ar	3.5	246.0	298.0	498.0	145.0
550	*p*-Nitrobenzyl alcohol	2.22 Ar	3.5	229.0	310.0	456.0	56.8
551	*p*-Nitrobenzyl chloride	2.22 Ar	3.5	278.0	307.0	466.0	110.0
552	2-Nitrobiphenyl	1.35 Ar	3.5	381.0	391.0	281.0	40.0
553	*o*-Nitrochlorobenzene	1.58 Ar	3.5	345.0			
554	*m*-Nitrocinnamic acid	2.46 Ar	3.5	268.0	319.0	512.0	42.0
555	*o*-Nitrocinnamic acid	2.50 Ar	3.5	256.0	298.0	742.0	81.3
556	*p*-Nitrocinnamic acid	2.43 Ar	3.5	301.0	310.0	626.0	67.2
557	4-Nitro-*m*-cresol	1.44 Ar	3.5	234.0	270.0	539.0	68.0
558	Nitrofurazone	0.90 Ar	3.5	216.2	233.9	519.7	∞
559	Nitroguanidine	1.46 Ar	3.5	183.9	214.1	223.0	∞
560	Nitromethane	1.59 Ar	3.5				
561	α-Nitronaphthalene	1.76 Ar	3.5		393.5	420.7	330.8
562	*p*-Nitrophenetole	2.42 Ar	3.5	335.0	350.0	386.0	26.0
563	*m*-Nitrophenol	2.45 Ar	3.5	297.0	353.0	486.0	137.0
564	*o*-Nitrophenol	2.34 Ar	3.5	275.0	300.0	212.0	32.7
565	*p*-Nitrophenol	2.51 Ar	3.5	268.0	302.0	399.0	19.4
566	*p*-Nitrophenol sodium salt	1.40 Ar	3.5	296.0			
567	*m*-Nitrophenylacetic acid	2.17 Ar	3.5	232.0	274.0	473.0	22.4
568	*o*-Nitrophenylacetic acid	2.59 Ar	3.5	218.0	243.0	231.0	28.3
569	*p*-Nitrophenylacetic acid	2.31 Ar	3.5	244.0	275.0	350.0	34.8
570	4-Nitrophenyl disulfide	1.42 Ar	3.5	160.0	248.0	467.0	18.2
571	4-Nitrophenylhydrazine	1.11 Ar	3.5	159.0	178.0	432.0	25.8
572	*o*-Nitrophenylhydrazine	1.70 Ar	3.5	165.0	186.0	595.0	898.0
573	4-Nitrophenylphosphoro dichloridate	1.80 Ar	3.5	178.0	316.0	1022.0	∞
574	*o*-Nitrophenylsulfenyl chloride	1.15 Ar	3.5	122.0	169.0	434.0	15.0
575	1-Nitropropane	1.57 Ar	3.5				
576	6-Nitroquinoline	1.01 Ar	3.5	339.8	378.8	338.8	35.7
577	*N*-Nitrosodimethylamine	1.00 Ar	3.5	333.0	343.0	36.0	5.2
578	*N*-Nitrosodiphenylamine	1.13 Ar	3.5				
579	2-Nitroso-5-(*N*-ethyl-*N*-sulfopropylamino)phenol	1.48 Ar	3.5	144.0	189.0	157.0	∞
580	5-Nitroso-8-hydroxyquinoline	1.23 Ar	3.5	211.0	243.0	255.0	∞
581	*N*-[*N*-Nitrosomethylamino)methyl]benzamide	1.35 Ar	3.5	134.0	134.0	392.0	∞
582	*N*-Nitrosomethylurea	~1 Ar	3.5	66.0		316.0	
583	α-Nitroso-β-naphthol	1.64 Ar	3.5	115.0	140.0	275.0	133.0
584	β-Nitroso-α-naphthol	1.21 Ar	3.5	134.0	155.0	154.0	853.0
585	*p*-Nitrosophenol	1.34 Ar	3.5				

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min^2 g)
586	2-Nitroso-5-(*N*-propyl-*N*-sulfopropylamino)phenol	1.78 Ar	3.5	186.0	208.0	104.0	∞
587	5-Nitrosothiobarbituric acid	1.55 Ar	3.5	140.0	186.0	120.0	74.0
588	2-Nitro-5-thiocyanatobenzoic acid	1.27 Ar	3.5	161.0	254.0	524.0	22.6
589	*m*-Nitrotoluene	2.45 Ar	3.5	332.0	361.0	260.0	25.0
590	*o*-Nitrotoluene	2.37 Ar	3.5	317.0	338.0	317.0	17.2
591	*p*-Nitrotoluene	2.41 Ar	3.5	332.0	366.0	372.0	141.0
592	*p*-Nitro-*o*-toluidine	1.47 Ar	3.5	290.0	329.0	481.0	250.0
593	3-Nitro-1*H*-1,2,4-triazole	1.18 Ar	3.5	237.3	200.3	264.8	3.3
594	5-Nitrouracil	0.98 Ar	3.5	299.7	303.4	465.1	∞
595	5-Nitrovanillin	1.89 Ar	3.5	184.0	198.0	548.0	13.7
596	1-Octene	1.46 Ar	3.5				
597	n-Octyl aldehyde	1.51 Ar	3.5				
598	*t*-Octyl disulfide	1.50 Ar	3.5				
599	Orcinol	1.59 Ar	3.5				
600	Oxalyl dihydrazide	1.22 Ar	3.5	244.0	247.5	435.7	115.6
601	Palmitoyl chloride	1.40 Ar	3.5	245.0	234.0	305.0	80.0
602	Parathion	1.54 Ar	3.5	208.0	269.0	480.0	484.0
603	Pentaerythritol tetranitrate	1.45 Ar	3.5	163.0	197.0	764.0	330.0
604	3-Pentanone	1.18 Ar	3.5				
605	2-Pentene	1.53 Ar	3.5				
606	Phenaceturic acid	1.51 Ar	3.5				
607	Phenazine	1.35 Ar	3.5				
608	Phenethyl acetate	1.24 Ar	3.5				
609	Phenol	1.43 Ar	3.5	233.0	249.0	542.0	281.0
610	Phenoxazine	1.37 Ar	3.5				
611	2-(2-Phenylacetamido)acetaldoxime	1.26 Ar	3.5	150.0	157.0	279.0	47.8
612	Phenylacetoaldehyde	1.91 Ar	3.5				
613	Phenylacetonitrile	1.61 Ar	3.5				
614	3-Phenylacetylacetone	1.79 Ar	3.5				
615	Phenylalanine	1.84 Ar	3.5				
616	*N*-Phenylanthranilic acid	1.32 Ar	3.5				
617	Phenylazoformic acid-2-phenylhydrazide	1.28 Ar	3.5	162.0	162.0	314.0	∞
618	*p*-Phenylene diisothiocyanate	1.73 Ar	3.5	386.0	400.0	78.3	13.3
619	D,L-2-Phenyl glycine	1.45 Ar	3.5				
620	1-Phenylheptane	1.92 Ar	3.5				
621	Phenylhydrazine	1.64 Ar	3.5	239.0	295.0	144.0	12.2
622	Phenylhydrazine-*p*-sulfonic acid	1.82 Ar	3.5	279.0	291.0	74.8	∞
623	Phenylisothiocyanate	1.31 Ar	3.5				
624	L-3-Phenyl lactic acid	1.76 Ar	3.5				
625	1-Phenyl-5-mercapto-1*H*-tetrazole	1.85 Ar	3.5	150.0	152.0	284.0	∞
626	Phenylmethylsulfonyl fluoride	1.56 Ar	3.5	285.0	285.0	11.1	44.7
627	3-Phenylpropionaldehyde	1.65 Ar	3.5				
628	3-Phenylpropionyl chloride	1.42 Ar	3.5	182.0	203.0	987.0	364.0
629	1-Phenylsemicarbazide	1.77 Ar	3.5	207.0	217.0	204.0	
630	Phenyl sulfide	1.56 Ar	3.5				
631	Phenyl sulfoxide	1.72 Ar	3.5	346.0	364.0	110.0	12.5
632	1-Phenyl-2-thiourea	1.81 Ar	3.5	236.0	253.0	72.0	4.8
633	Phenylurea	1.86 Ar	3.5				
634	Phenyl vinyl sulfoxide	1.54 Ar	3.5	232.0	251.0	319.0	112.0
635	Phthalazine	1.30 Ar	3.5	293.4	305.8	241.9	7.9

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min^2 g)
636	γ-Picoline	1.13 Ar	3.5				
637	γ-Picoline-*N*-oxide	1.51 Ar	3.5	242.0	285.0	368.0	161.0
638	Picolinic acid *N*-oxide	1.27 Ar	3.5	259.0	307.0	224.0	24.8
639	Pimelic acid	1.44 Ar	3.5				
640	Pinacoline	1.57 Ar	3.5				
641	4-Pipecoline	1.63 Ar	3.5				
654	Pierazine-*N,N'*-bis(2-ethane sulfonic acid)	1.36 Ar	3.5				
643	Piperidine	1.91 Ar	3.5				
644	Piperonal	0.97 Ar	3.5	330.0	363.3	143.3	7.6
645	1,3-Propanediamine	1.62 Ar	3.5				
646	Propionaldehyde	1.62 Ar	3.5				
647	Propionamide	1.59 Ar	3.5				
648	Propionitrole	1.84 Ar	3.5				
649	n-Propylamine	1.33 Ar	3.5				
650	n-Propyl benzoate	1.95 Ar	3.5				
651	n-Propyl gallate	1.31 Ar	3.5	358.0	364.0	21.0	35.0
652	n-Propyl mercaptan	1.68 Ar	3.5				
653	n-Propyl propionate	1.92 Ar	3.5				
654	2-Propyn-1-ol	1.12 Ar	3.5				
655	Purine	1.18 Ar	3.5		328.7	90.7	7.1
656	Pyrazine	1.08 Ar	3.5				
657	Pyrazole	1.72 Ar	3.5				
658	Pyridazine	1.81 Ar	3.5				
659	Pyridine	1.22 Ar	3.5				
660	*syn*-2-Pyridine aldoxime	1.31 Ar	3.5	207.2	235.2	417.9	169.6
661	2-Pyridinecarbaldehyde oxime	1.16 Ar	3.5	214.2	242.6	372.8	118.0
662	Pyridine *N*-oxide	1.33 Ar	3.5	251.0	288.0	380.0	53.9
663	3-(2-Pyridyl)-5,6-diphenyl-1,2,4-triazine	1.12 Ar	3.5				
664	2-Pyridylhydroxymethanesulfonic acid	1.37 Ar	3.5	227.0	243.8	129.1	57.9
665	Pyrocatechol	1.89 Ar	3.5	365.0	367.0		
666	Pyruvic acid	1.86 Ar	3.5	130.2	159.0	134.2	∞
667	Quinaldine	1.48 Ar	3.5				
668	Quinoline	1.68 Ar	3.5				
669	Rhodanine	1.01 Ar	3.5				
670	Salicylaldoxime	1.65 Ar	3.5	192.0	249.0	379.0	285.0
671	Salicylhydrazide	1.35 Ar	3.5	209.0	231.0	178.0	2.1
672	Salicylhydroxamic acid	1.53 Ar	3.5	175.0	175.0	559.0	∞
673	Sebacoyl dihydrazide	1.56 Ar	3.5				
674	Stearanilide	1.43 Ar	3.5				
675	Styrene, monomer	1.76 Ar	3.5				
676	Styrene oxide	1.85 Ar	4.9		273.0	107.0	21.0
677	Succinamide	1.51 Ar	3.5				
678	Succinic anhydride	1.61 Ar	3.5	342.4	347.8	36.7	13.6
679	5-Sulfosalicylic acid, dihydrate	1.67 Ar	3.5				
680	Taurine	1.58 Ar	3.5				
681	Taurocyamine	1.09 Ar	3.5				
682	α,α,α',α'-Tetrabromo-*o*-xylene	1.71 Ar	3.5	301.0	332.0	398.0	503.0
683	Tetrahydrofurfuryl alcohol	1.48 Ar	3.5				
684	Tetrahydro-2-methylfuran	1.42 Ar	3.5				
685	*cis*-Δ^4-Tetrahydrophthalic anhydride	1.25 Ar	3.5				

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min^2 g)
686	*cis*-1,2,3,6-Tetrahydrophthalimide	1.15 Ar	3.5				
687	Tetrahydropyran	1.71 Ar	3.5				
688	Tetralin	0.94 Ar	3.5				
689	1-Tetralone	1.32 Ar	3.5				
690	1*H*-Tetrazole	1.67 Ar	3.5	170.2	206.6	937.1	94.5
691	Thioanisole	1.12 Ar	3.5				
692	*S*-(Thiobenzoyl)thioglycolic acid	1.64 Ar	3.5	193.0	209.0	40.7	3.5
693	Thiocarbohydrazide, crsytal	1.32 Ar	3.5	179.0	179.0	460.0	∞
694	Thiocarbonohydrazide	1.19 Ar	3.5	172.6	174.0	374.1	∞
695	*m*-Thiocresol	1.31 Ar	3.5	134.0	223.0	258.0	2.2
696	*p*-Thiocresol	1.31 Ar	3.5				
697	D,L-Thioctic acid	1.26 Ar	3.5				
698	Thiodiglycolic acid	1.28 Ar	3.5	288.3	306.0	108.4	9.8
699	Thiophene	1.20 Ar	3.5				
700	2-Thiophene carboxylic hydrazide	1.19 Ar	3.5	270.0	316.7	144.1	36.2
701	Thiourea	1.42 Ar	3.5	304.7	317.9	76.0	∞
702	Thymol	1.47 Ar	3.5	296.0	302.0	239.0	273.0
703	*o*-Toluenesulfonamide	1.21 Ar	3.5	374.0	374.0	40.0	180.0
704	*p*-Toluenesulfonamide	1.58 Ar	3.5	374.0	376.0	75.2	∞
705	4-Toluenesulfonyl chloride	1.20 Ar	3.5	282.0	292.0	362.0	∞
706	*p*-Toluenesulfonyl fluoride	1.58 Ar	3.5				
707	*m*-Tolunitrile	1.67 Ar	3.5				
708	*p*-Tolylthiophosphonic dichloride	1.64 Ar	3.5	160.0	162.0	323.0	21.0
709	1,2,4-Triacetoxybenzene	1.33 Ar	3.5	357.0	378.0	52.4	37.4
710	Triacetylmethane	1.42 Ar	3.5				
711	2,4,6-Triamino-1,3,5-triazine	1.51 Ar	3.5				
712	Tribenzylamine	1.38 Ar	3.5				
713	2,4,6-Tribromoaniline	1.52 Ar	3.5	367.0	454.0	279.0	∞
714	2,2′,4′-Trichloroacetophenone	1.55 Ar	3.5	305.0	316.0	574.0	∞
715	2,4,5-Trichloroaniline	1.62 Ar	3.5	388.0	436.0	402.0	∞
716	2,4,5-Trichlorobenzenesulfonyl chloride	1.57 Ar	3.5				
717	2,4,5-Trichlorobenzenesulfonyl hydrazide	1.28 Ar	3.5	114.0	124.0	608.0	381.0
718	2,4,5-Trichlorophenol	1.35 Ar	3.5	253.0	268.0	699.0	∞
719	2,4,5-Trichlorophenoxyacetic acid	1.45 Ar	3.5	350.0	383.0	676.0	∞
720	2,4,5-Trichlorophenyl disulfide	1.73 Ar	3.5	348.0	355.0	330.0	298.0
721	Tricresyl phosphate	1.48 Ar	3.5				
722	α,α,α-Trifluoro-2,6-dinitro-*N*,*N*-dipropyl-*p*-toluidine	1.36 Ar	3.5	212.0	256.0	657.0	29.5
723	α,α,α-Trifluoro-o-tolylisocyanate	1.22 Ar	3.5				
724	2,4,5-Trihydroxypyrimidine	1.25 Ar	3.5				
725	2,4,6-Triiodophenol	1.55 Ar	3.5	367.0	380.0	170.0	37.0
726	2,3,4-Trimethoxybenzaldehyde	1.36 Ar	3.5	354.0	367.0	234.0	8.4
727	2,3,4-Trimethoxybenzoic acid	1.15 Ar	3.5	330.0	351.0	216.0	3.7
728	2,4,5-Trimethoxybenzoic acid	1.72 Ar	3.5	357.0	380.0	214.0	10.0
729	3,4,5-Trimethoxycinnamic acid	1.89 Ar	3.5	285.0	382.0	227.0	12.1
730	2′,4′,6′-Trimethylacetophenone	1.16 Ar	3.5				
731	Trimethylamine *N*-oxide, dihydrate	1.31 Ar	3.5	152.0	202.0	213.0	76.6
732	2,4,5-Trimethylaniline	1.37 Ar	3.5				
733	2,4,6-Trimethylbenzyl alcohol	1.53 Ar	3.5				
734	1,3,5-Trimethylcyclohexane	1.16 Ar	3.5				
735	2,3,5-Trimethylphenol	1.41 Ar	3.5	279.0	290.0	256.0	203.0

TABLE 3 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min² g)
736	2,4,6-Trinitrotoluene	1.46 Ar	3.5	273.0	314.0	1287.0	∞
737	Triphenyl phosphate	1.18 Ar	3.5				
738	Triphenyl phosphine	1.93 Ar	3.5				
739	Triphenyl phosphine oxide	1.79 Ar	3.5				
740	Triphenyl phosphine sulfide	1.73 Ar	3.5				
741	*N*-tris(Hydroxymethyl)methyl-2-aminoethane sulfonic acid	1.68 Ar	3.5	230.3	231.5	84.9	14.4
742	Tropaeolin O	1.27 Ar	3.5	239.0	252.0	120.0	13.5
743	Tropic acid	1.81 Ar	3.5	220.0	270.0	76.1	11.1
744	10-Undecenal	1.72 Ar	3.5				
745	Uracil	1.02 Ar	3.5				
746	Urea	1.25 Ar	3.5				
747	n-Valeramide	1.29 Ar	3.5				
748	2-Vinylpyridine	1.51 Ar	3.5	184.0	190.0	79.8	4.1
749	Xanthene	1.20 Ar	3.5				
750	Xanthone	1.14 Ar	3.5				
751	Xanthurenic acid	1.56 Ar	3.5	351.7	343.0	41.9	1.6
752	3,4-Xylyl-*N*-methylcarbamate	1.48 Ar	3.5				

imes (471 cal/g) and azoxy compounds (445 cal/g). However, some values for the acid chlorides are not reliable as the compounds react exothermically with the aluminum cell.

4. Conclusion

Differential scanning calorimetry experiments for 820 reactive chemicals with various functional groups were conducted to assess the possibility of using DSC data to classify compounds in accordance with their thermal hazards. Exothermic onset temperatures (T_o) and heats of decomposition (Q), which correspond to sensitivity and severity, respectively, were evaluated as independent factors because between them the correlation coefficient was low and a wide distribution of values was obtained. It is possible to classify the thermal hazards of reactive chemicals in a two-dimensional representation in terms of T_o and Q.

It has also become apparent that the proportion of exothermically decomposed samples and the mean values of T_o and Q for reactive chemicals may be dependent on the functional groups in the compounds.

Thus, although it was found to be possible to make a rough estimation of thermal hazards for reactive chemicals by DSC experiments, a statistical method such as multivariate analysis, in which kinds, number and position of

TABLE 4

Thermal data for some chemcials as obtained with the sealed SUS cell

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min^2 g)
1	Acetaldoxime	1.00 Air	0.1				
2	5-Acetylamino-1,2,3-thiadiazole	0.64 N_2	0.1	209.0		131.1	
3	2-Amino-3-chloro-1,4-naphthoquinone	1.56 Air	0.1	285.0	302.0	195.0	327.0
4	3-Amino-2-chloropyridine	1.31 Air	0.1	277.0	284.0	242.0	∞
5	5-Amino-2-chloropyridine	1.39 Air	0.1	271.0	295.0	302.0	71.8
6	2-Amino-3,5-dibromopyridine	1.38 Air	0.1	288.0	321.0	265.0	333.0
7	4-Amino-1,3-dimethyl-2,6-dioxy-5-nitrosopyrimidine	1.08 Air	0.1	184.0	223.0	262.0	694.0
8	5-Amino-1,2,3-thiadiazole	0.58 N_2	0.1	151.0		281.6	
9	Azobenzene	1.52 Air	0.1	379.0		162.0	
10	2,2′-Azobis-2,4-dimethylvaleronitrile	0.60 Air	0.1	63.0		303.1	
11	2,2′-Azobisisobutyronitrile	0.55 Air	0.1	102.5		356.5	
12	Azoxybenzene	1.92 Air	0.1	241.0		329.0	
13	Benzenazodiphenylamine	1.17 Air	0.1	324.0	358.0	128.0	21.0
14	1,3,5-Benzenetricarboxylic acid chloride	1.31 Air	0.1	420.0	440.0		22.9
15	Benzophenonehydrazone	1.08 Air	0.1	310.0	334.0	230.0	6.1
16	Benzoyl peroxide	1.09 Air	0.1	113.0		369.0	
17	Bleaching powder	2.73 Air	0.1	192.0		100.8	
18	2-Bromo-n-butyric acid	1.60 Air	0.1	106.0	116.0	263.0	33.3
19	α-Bromo-γ-butyrolactone	1.75 Air	0.1	184.0	212.0	172.0	87.4
20	2-Bromo-2-cyano-*N,N*-dimethylacetamide	1.67 Air	0.1				
21	5-Bromocytosine	1.41 Air	0.1	240.0	255.0	174.0	203.0
22	*N*-(2-Bromoethyl)phthalimide	1.58 Air	0.1	309.0	346.0	113.0	242.0
23	2-Bromothiazole	1.40 Air	0.1	200.0	240.0	395.0	∞
24	Capryl chloride	1.09 Air	0.1	210.0	215.0	217.0	220.0
25	2-Chloroacetamide	1.44 Air	0.1	155.0	193.0	503.0	106.0
26	Chlorobenzene	1.42 Air	0.1				
27	5-Chloro-2-methyl-4-isothiazoline-3-one	1.50 Air	0.1	191.0	209.0	287.0	∞
28	2-Chloro-5-nitropyridine	1.52 Air	0.1	322.0	322.0	687.0	∞
29	5-Chloro-2-n-octyl-4-isothiazoline-3-one	1.65 Air	0.1	186.0	195.0	210.0	464.0
30	6-Chloropurine	1.39 Air	0.1	179.0	179.0	16.3	∞
31	5-Chloro-3-pyridinol	1.23 Air	0.1	285.0	299.0	310.7	63.2
32	2-Chloroxanthone	1.26 Air	0.1	442.0	472.0	203.0	146.0
33	Congo Red	1.00 Air	0.1	284.0	296.0	65.0	39.4
34	Cyclohexyl bromide	1.40 Air	0.1	156.5	156.5	115.7	10.8
34	1,1-Dibromoethane	1.12 Air	0.1				
36	5,7-Dibromo-8-hydroxyquinoline	1.48 Air	0.1	213.6	213.6	158.3	16.7
37	2,6-Dibromopyridine	1.50 Air	0.1	367.0	372.0	270.0	∞
38	Dichloroacetic acid	1.48 Air	0.1				
39	1,4-Dichlorobutane	1.41 Air	0.1	355.4	359.7	79.3	23.2
40	4,5-Dichloro-2-methyl-4-isothiazoline-3-one	1.49 Air	0.1	266.0	290.0	375.0	∞
41	2,3-Dichloro-1,4-naphthoquinone	1.59 Air	0.1	366.9	394.2	128.8	41.7
42	4,5-Dichloro-2-n-octyl-4-isothiazoline-3-one	1.65 Air	0.1	228.0	243.0	265.0	500.0
43	1,3-Dichloropropane	1.35 Air	0.1	234.4	242.6	81.4	12.4
44	2,5-Dichlorothiophene	1.33 Air	0.1	261.0	281.0	34.1	5.0
45	3,5-Dinitro-4-chlorobenzotrifluoride	1.00 Air	0.1	160.0	160.0	71.0	420.0
46	Dinitrosopentamethylenetetramine	0.57 Air	0.1	166.0		493.4	
47	3,5-Dinitro-*o*-toluic acid	1.25 Air	0.1	267.0		458.0	
48	Diphenyl carbamoyl chloride	1.54 Air	0.1	270.0	295.0	453.0	5.1
49	1,2-Epoxypropane	1.34 Air	0.1	159.0	160.0	67.0	582.0
50	2,3-Epoxy-1-propanol	1.46 Air	0.1	115.0		441.0	

TABLE 4 (continued)

Chemicals		Procedure		Thermal data			
No.	Name	Weight gas (mg)	Pressure (MPa)	T_a (°C)	T_o (°C)	Q (cal/g)	V (cal/min² g)
51	2,3-Epoxy-1-propyl methacrylate	1.27 Air	0.1	155.0	155.0	149.0	472.0
52	Ethyl bromoacetate	1.50 Air	0.1	296.2	331.1	127.9	132.0
53	Ethylene cyanohydrin	1.36 Air	0.1				
54	1-Ethyl-3-*p*-tolyltriazine	1.03 Air	0.1	90.0	103.0	179.0	14.6
55	Ethyl trifluoroacetate	1.14 Air	0.1				
56	*S*-Ethyl trifluorothioacetate	1.14 Air	0.1				
57	2-Fluoropyridine	1.51 Air	0.1				
58	Formamide	1.43 Air	0.1				
59	*N*-Formylmorpholine	1.23 Air	0.1				
60	1,2,3,4,5,6-Hexachlorocyclohexane	1.42 Air	0.1				
61	1,5-Hexadiene	1.22 Air	0.1				
62	1,1,1,3,3,3-Hexafluoro-2-propanol	2.30 Air	0.1				
63	Hydrazobenzene	1.41 Air	0.1	179.0		40.0	
64	1-(1-Hydroxy-4-methyl-2-phenylazo)-2-naphthol-4-sulfonic acid	1.27 Air	0.1	155.0	155.0	112.0	101.0
65	4-(8-Hydroxy-5-quinolylazo)naphthalene-1-sulfonic acid	1.10 Air	0.1	253.0	269.0	265.0	150.0
66	*o*-{2-[α-(Hydroxy-5-sulfophenylazo)benzylidene]hydrazino}benzoic acid, Na-salt	1.24 Air	0.1	221.0	227.0	148.0	15.5
67	2-Hydroxy-5-trifluoromethylpyridine	1.42 Air	0.1	227.0	240.1	112.5	8.9
68	Iodoform	1.24 Air	0.1	265.0	277.0	162.0	33.7
69	Isoamyl nitrite	1.44 Air	0.1	109.0		727.0	
70	Isophthaloyl chloride	1.00 Air	0.1	400.0	405.0	262.0	90.0
71	4-Methoxybenzyloxycarbonylazide	1.00 Air	0.1	114.0	132.0	291.0	24.0
72	Methoxycarbonyl chloride	1.08 Air	0.1				
73	4-Methyl-3-nitrobenzoic acid	1.14 Air	0.1	160.0	160.0	234.0	526.0
74	2-Methyl-4,4,5,5-tetrachloroisothiazolizine-3-one	1.55 Air	0.1	200.0	204.0	114.0	11.8
75	Mucochloric acid	1.32 Air	0.1	246.9	263.4	216.5	22.3
76	Naphthanyldiazo Blue B	1.00 Air	0.1	105.0	132.0	103.0	
77	Naphthanyldiazo Red RC	1.10 Air	0.1	160.0	160.0	110.0	464.0
78	Neurine bromide	1.14 Air	0.1	139.4	162.8	265.9	18.2
79	*p*-Nitrobenzenediazoniumtetrafluoroborate	1.06 Air	0.1	135.0	150.0	140.0	00
80	*N*-Nitrosomethylurea	1.12 Air	0.1	90.0	103.0	285.0	201.0
81	2-n-Octyl-4-isothiazoline-3-one	1.41 Air	0.1	242.0	264.0	139.0	540.0
82	2-n-Octyl-4,4,5,5-tetrachloroisothiazolizine-3-one	1.49 Air	0.1	212.0	251.0	234.0	49.7
83	4,4′-Oxybis(benzensulfonylhydrazide)	0.60 Air	0.1	146.0		207.4	
84	α-Picoline-*N*-oxide	1.08 Air	0.1	255.0	291.0	498.0	72.2
85	β-Picoline-*N*-oxide	1.25 Air	0.1	160.0	160.0	73.0	600.0
86	Pyridine *N*-oxide	1.21 Air	0.1	236.0		365.0	
87	4-(2-Pyridylazo)resorcinol	1.14 Air	0.1	180.0	198.0	110.0	895.0
88	Stilbene-4,4′-bis[(1-azo)-3,4-dihydroxybenzene]-2,2-disulfonic acid diammonium	1.15 Air	0.1	202.0	218.0	64.0	5.4
89	Sudan III	1.00 Air	0.1	237.0	279.0	367.0	25.5
90	Tetrabromoethane	1.53 Air	0.1				
91	1,1,2,2-Tetrachloroethane	1.14 Air	0.1				
92	Tetrachloroethylene	1.31 Air	0.1				
93	2-(2-Thiazolylazo)-*p*-cresol	1.00 Air	0.1	247.0	264.0	264.0	780.0
94	1-(2-Thiazolylazo)-2-naphthol	1.41 Air	0.1	190.0	230.0	186.0	209.0
95	*p*-Toluenesulfonyl hydrazide	0.58 Air	0.1	124.0		253.8	
96	1,2,3-Tribromopropane	1.38 Air	0.1				
97	Trimethylacetyl chloride	1.24 Air	0.1	81.0	115.0	63.0	34.2

the functional groups are considered, may be necessary to make more exact assessments.

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