

Prediction of explosibility of self-reactive materials by calorimetry of a laboratory scale and thermochemical calculations

Yoshihiko Sato^{*†}, Miyako Akiyoshi^{*}, Atsumi Miyake^{**}, and Takehiro Matsunaga^{*}

^{*}Research Core for Explosion Safety, Research Institute of Science for Safety and Sustainability (RISS), National Institute of Advanced Industrial Science and Technology (AIST),
AIST Tsukuba Central 5, 1-1-1 Higashi, Tsukuba-shi, Ibaraki 305-8565, JAPAN
TEL : +81-29-861-4785

[†]Corresponding address : yoshihiko-satou@aist.go.jp

^{**}Graduate School of Environment and Information Sciences, Yokohama National University,
79-7 Tokiwadai, Hodogaya-ku, Yokohama 240-8501, JAPAN

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Abstract

Experimental results of accelerating rate calorimeter (ARC) and calculation results by the ASTM Chemical Thermodynamic and Energy Release Evaluation Program (CHETAH) were compared with literature data obtained from explosion propagation tests (BAM 50/60 steel tube tests or UN gap tests) in order to safely predict the explosibility of self-reactive materials. There is a mutual correlation between CHETAH criteria and the explosibility of self-reactive substances except in the cases of organic peroxides and azo compounds. There is also mutual correlation between maximum pressure per unit mol of substances measured by ARC and the explosibility of substances. Additionally, the temperature at maximum pressure rising rate is correlated with the explosibility of substances except in the case of nitro compounds. Consequently, the explosibility of self-reactive materials can be predicted by temperature and pressure measurements using ARC.

Keywords : explosibility, prediction, accelerating rate calorimeter, thermochemical calculations.

1. Introduction

Self-reactive substances that have characteristic bonding groups, for example, organic peroxides, nitro compounds, and azo compounds, are not only used as explosives but also as raw materials for medicines and reaction accelerators. It is clear that these substances are valuable from an industrial point of view. However, since these substances may ignite and decompose vigorously by heat or shock even in the absence of air or oxygen, they are potentially quite hazardous. These explosive hazards can be estimated by applying standard test methods¹⁾. However, the standard tests require a large amount of sample and multiple tests must be performed. Therefore, it is not realistic to conduct these tests at the initial stages of development of a new substance. With respect to safety,

procurement of samples, and cost, it is desirable that the explosibility of self-reactive compounds can be evaluated safely by simple methods.

Predicting heat of decomposition by a calculation technique is an important means of estimating explosive hazards. Thermochemical calculations and chemical equilibrium calculations are applied to estimate the heat of decomposition of self-reactive materials. In particular, thermochemical calculations are frequently applied due to their light calculation load²⁾. The heat of formation is required to predict the heat of decomposition by calculations. This can be obtained by measuring the heat of combustion³⁾. However, in the case of unknown self-reactive substances, there is a danger of explosive accidents when measuring the heat of combustion. Thus,

many authors have attempted to estimate the heat of formation of chemical materials using calculation techniques^{4)–15)}. Among them, Benson⁴⁾ has proposed estimating the heat of formation using additivity rules. Benson's technique was introduced to the CHETAH (Chemical Thermodynamic and Energy Release) program developed by ASTM (American Society for Testing and Materials)¹⁶⁾ and the REITP (Revised Estimation of Incompatibility from Thermochemical Properties) program developed by the University of Tokyo¹⁷⁾. It should be noted that the estimated heat of formation by calculations is the gas phase value at a standard state. Thus, in most cases, this value cannot be applied to self-reactive substances because the substances are generally in the condensed phase at a standard state. In order to overcome this difficulty, Ijichi and Matsunaga have proposed group contributions to the heat of formation of condensed states and mentioned that the agreement between the calculated and observed heats of formation is sufficient to estimate the hazardous properties of energetic materials^{6),7)}. However, the correlation between the energy release factors, such as heat of decomposition, and the results of the explosion propagation tests has not been evaluated. This must be done in order to evaluate the adequacy of prediction using thermochemical calculations.

Alternatively, differential scanning calorimetry is generally used to determine the heat of decomposition experimentally^{18),19)}. However, Whitmore has pointed out that this energy screen is often overly conservative because it is based only on internal energy. In other words, the energy change due to molecular fragmentation and gas evolution is neglected²⁰⁾. In order to solve this problem, many authors have proposed measuring pressure and/or rate of pressure rise data using closed pressure vessel tests as a screening technique for explosive properties^{20)–23)}. We noted that an accelerating rate calorimeter (ARC) could measure not only temperature data but also pressure data. ARC has been generally applied to measurements of the thermal sensitivity of self-reactive substances accurately under adiabatic conditions. Thus, ARC has mainly been applied to runaway reactions by thermal accumulations. On the other hand, ARC measures not only an adiabatic temperature rise by exothermic decomposition under adiabatic conditions but also a pressure rise under closed conditions. Therefore, ARC may estimate not only heat of decomposition but also the energy change due to molecular fragmentation and gas evolution, the parameters associated with the explosibility of substances.

In this study, in order to investigate the adequacy of predicting the explosibility of substances using a thermochemical calculation technique, the correlation between estimated criteria using CHETAH and results from explosion propagation tests was investigated using measured heats of formation and heats of formation calculated by additivity rules. Moreover, in order to evaluate the possibility of predicting the explosibility of substances by measuring these values by ARC, the correlation between the measured temperature and

pressure data using ARC and the results of explosion propagation tests was determined.

2. Experiments and calculations

2.1 Materials

Table 1 shows the samples used in this study. The "Explosibility" column in Table 1 shows results of BAM 50/60 steel tube tests¹⁾ and UN gap tests²⁴⁾ on each sample. All chemical reagents are analytical grade and were used without further purification.

2.2 Measurements using ARC adiabatic calorimeter

ARC measurements were conducted using New ARC (TIAx). The measurements were performed using the Heat-Wait-Search mode¹⁹⁾ starting at 50°C and incrementing by 5°C. The waiting and searching times were both 15 min. The heating rate was 5K min⁻¹. A 9-mL nickel-chromium alloy (Hastelloy-C) sample vessel with an upper tube of 6.35 mm in diameter was used. The weight of the vessel was about 20 g. A heating capacity of the ARC heater is known to be about 10 K min⁻¹. Thus, the amount of sample was arranged such that the self-heating rate was not faster than the heating capacity of the ARC heater. Table 1 also shows these amounts.

2.3 Measurement of heat of combustion using a combustion calorimeter and calculation of heat of formation

The heat of combustion was measured using a C2000 basic combustion calorimeter (IKA). A C5012 bomb for resisting pressure and corrosion by halides was used. Approximately 0.25 g of sample was placed into a stainless steel crucible and the crucible was set in a crucible holder. A wire for ignition was attached to the electrodes of the bomb. Approximately 8 cm of cotton thread was tied to the middle position of the ignition wire and extended to the sample in the crucible, as shown in Fig. 1. The crucible was placed in the bomb and the screw cap of the bomb was closed. The bomb was placed into the calorimeter and 3 MPa of oxygen was filled into the bomb. The heat of combustion was measured by igniting the sample. The heat of combustion was defined as the averaged value of three measurements. Samples that burned incompletely were measured after mixing with liquid paraffin (Wako Chemicals) as a combustion improver. In these cases, the amount of sample was about 0.15 g and the combustion improver was about 0.2 g. The heat of formation was calculated by the following equation using the measured heat of combustion:

$$\Delta H_{comb} = \sum (\nu \times \Delta H_f^0)_{products} - \sum (\nu \times \Delta H_f^0)_{reactants}$$

where ΔH_{comb} is heat of combustion, ΔH_f^0 is heat of formation, and ν is its respective stoichiometric coefficient. It was assumed that the products were small stable compounds, such as water, CO₂, and N₂. Literature data²⁵⁾ was used for heats of formation of products.

Table 1 Samples chosen as subjects of this study.

No.	Substances	Abbreviation	Explosibility	The amount of samples for ARC[g]
1	Benzoyl peroxide ¹⁾	BPO	+ ⁵⁾ (BAM)	0.0513
2	Lauroyl peroxide ¹⁾	LPO	Partial (BAM)	1.0102
3	<i>tert</i> -Butyl peroxybenzoate ¹⁾	TBPB	Partial (BAM)	0.3553
4	Dicumyl peroxide ¹⁾	DPO	– ⁶⁾ (BAM)	0.6765
5	Cumene hydroperoxide ¹⁾	CHP	– (BAM)	0.3238
6	<i>tert</i> -Butyl hydroperoxide ¹⁾	TBHP	– (BAM)	0.7496
7	2,4-Dinitrotoluene ²⁾	DNT	+ (BAM)	0.2232
8	3,5-Dinitrobenzoic acid ²⁾	DNBA	+ (BAM)	–
9	2-Amino-4-chloro-5-nitrophenol ²⁾	5NPh	– (UN)	–
10	2-Bromo-2-nitro-1,3-propanediol ²⁾	2NP	+ (UN)	–
11	3-Nitrobenzenesulfonic acid sodium salt ²⁾	NBSA	– (UN)	–
12	2-Chloro-5-nitrobenzoic acid ²⁾	CNBA	+ (UN)	0.2678
13	4-Nitrophenylhydrazine ²⁾	NPH	+ (UN)	0.6808
14	2,2'-Azodiisobutyronitrile ³⁾	AIBN	+ (BAM)	0.1519
15	Azodicarbonamide ³⁾	ADCA	– (BAM)	0.1552
16	1-Phenyltetrazole-5-thiol ³⁾	5MT	– (UN)	–
17	<i>N,N'</i> -Dinitrosopentamethylenetetramine ⁴⁾	NNDNP	+ (BAM)	–
18	Ammonium nitrate ⁴⁾	AN	+ (BAM)	–
19	3-Thiosemicarbazide ⁴⁾	TSC	– (UN)	–

1) Organic peroxides

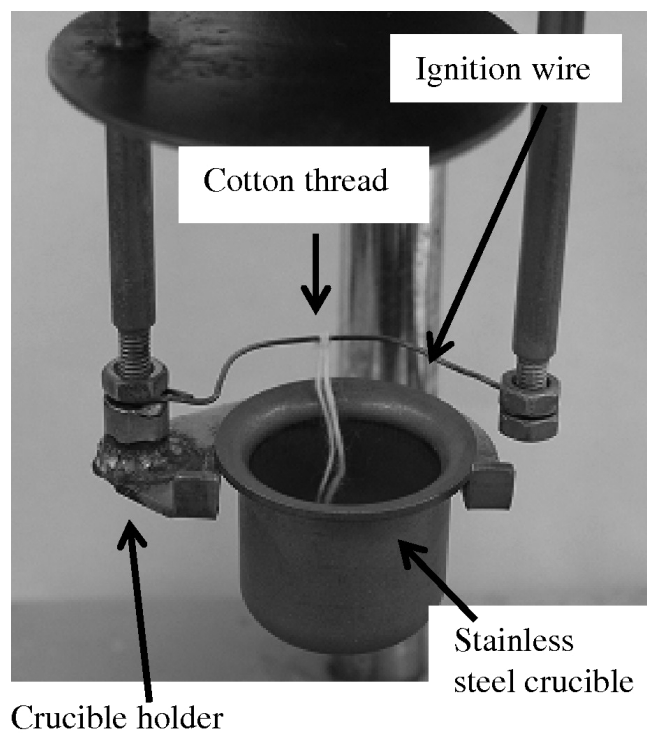
2) Nitro compounds

3) Azo compounds

4) Others

5) Explosion

6) No explosion

**Fig. 1** View around the stainless steel crucible at the combustion calorimeter.

2.4 Heat of formation and CHETAH criteria calculation by CHETAH

The energy release of self-reactive materials was estimated using CHETAH ver. 8.0⁶⁾. The heat of formation was predicted by CHETAH using additivity rules. As mentioned previously, the calculated heat of formation using additivity rules is the value in the gas phase, but self-reactive substances in this study are in the condensed phase in a standard state. Therefore, the heat of formation was calculated using group contributions to the heat of formation in a condensed state as proposed by Ijichi and Matsunaga^{6), 7)}. The CHETAH criteria value was calculated using the heat of formation by additivity rules and by the measured heat of combustion. The correlation between the CHETAH criteria value and literature data from explosion propagation tests was investigated. The heat of formation for some samples was difficult to estimate due to limitations in the thermochemical database of additivity rules. For these samples, the heat of formation was not calculated using the additivity rules.

3. Results and discussion

3.1 The correlation between CHETAH criteria and the explosibility of self-reactive substances

Figure 2 to 6 show the correlation of CHETAH criteria and the literature data from explosion propagation tests. In these figures, the numbers in the plot correspond to the numbers in Table 1. The red and blue lines represent the

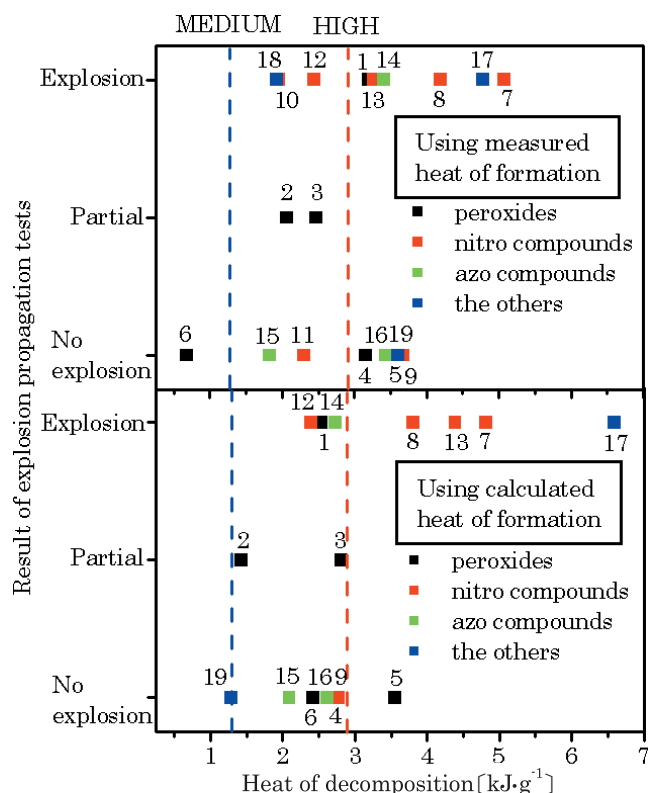


Fig. 2 The correlation of criterion 1 and literature data from explosion propagation tests.

“HIGH” and “MEDIUM” rating thresholds, respectively, as determined by CHETAH.

Criterion 1 concerns the maximum heat of decomposition¹⁶. Figure 2 shows the correlation of criterion 1 and the literature data from explosion propagation tests. The heats of decomposition of substances judged as “explosion” by explosion propagation tests tended to be lower than those of substances judged as “no explosion” by explosion propagation tests. Heats of decomposition of substances judged as “explosion” or “partial” by explosion propagation tests were greater than 1.3 kJ g^{-1} (0.3 kcal g^{-1}), the “MEDIUM” rating threshold by CHETAH. However, the heats of decomposition of seven substances judged as “no explosion” (4, 5, 9, 11, 15, 16, and 19) by explosion propagation tests were also larger than the “MEDIUM” rating threshold when using the measured heats of formation. When using the calculated heats of formation by additivity rules, the heats of decomposition of all seven substances judged as “no explosion” (4, 5, 6, 9, 15, 16, and 19) by explosion propagation tests were again greater than the “MEDIUM” rating threshold. If the heat of decomposition increases, it is likely that the energy utilized to propagate decomposition of the substances increases. Thus, it is reasonable to suppose that a relationship exists between heat of decomposition and the ease of propagation of decomposition. However, it is necessary to consider not only the ease of propagation of decomposition but also to include the expansion of produced gases in order to estimate the explosibility of a substance. Since gas quantity is unrelated to heat of decomposition, it is likely that considering only the heat of decomposition is not sufficient to estimate the explosibility of a substance. Accordingly, the heat of decomposition is a

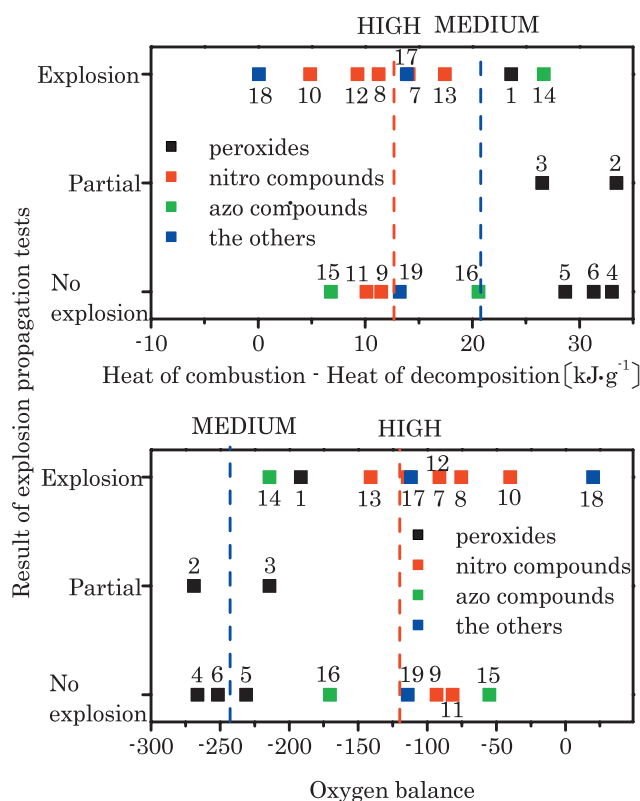


Fig. 3 The correlation of criteria 2 and 3 and literature data from explosion propagation tests.

tentative criterion for the explosibility of self-reactive substances, but it is difficult to estimate the explosibility of compounds using only this criterion.

Criterion 2 is a two-dimensional correlation that relates the difference between the maximum heat of decomposition and the heat of combustion¹⁶. Criterion 3 is the oxygen balance¹⁶. Since these criteria are determined by the number of elements in a molecule, they do not depend on the heat of formation. Figure 3 shows the correlation of criteria 2 and 3 and literature data from explosion propagation tests. Criterion 2 of two substances judged as “explosion” (1 and 14) by explosion propagation tests and two substances judged as “partial” (2 and 3) by explosion propagation tests was larger than 21 kJ g^{-1} (5 kcal g^{-1}), the “MEDIUM” rating threshold by CHETAH. Criterion 3 of one substance judged as “partial” (2) by explosion propagation tests was lower than -240 , the “MEDIUM” rating threshold by CHETAH. The difference between the maximum heat of decomposition and the heat of combustion, and the oxygen balance are indicators that show the ease of an intermolecular redox reaction²⁶. Thus, oxygen-rich compounds must be considered to have high explosibility. BPO, LPO, TBPB, and AIBN, judged as “explosion” or “partial” by explosion propagation tests, were rated “LOW” by these criteria, because it was clear that these compounds were fuel-rich compositions. Consequently, it is difficult to estimate the explosibility of substances by these criteria.

Criterion 4, Y , calculates a value defined as $Y = 10(M^2W/n)$, where M is the maximum heat of decomposition (criterion 1), W is the weight of the composition in grams, and n is the number of moles of

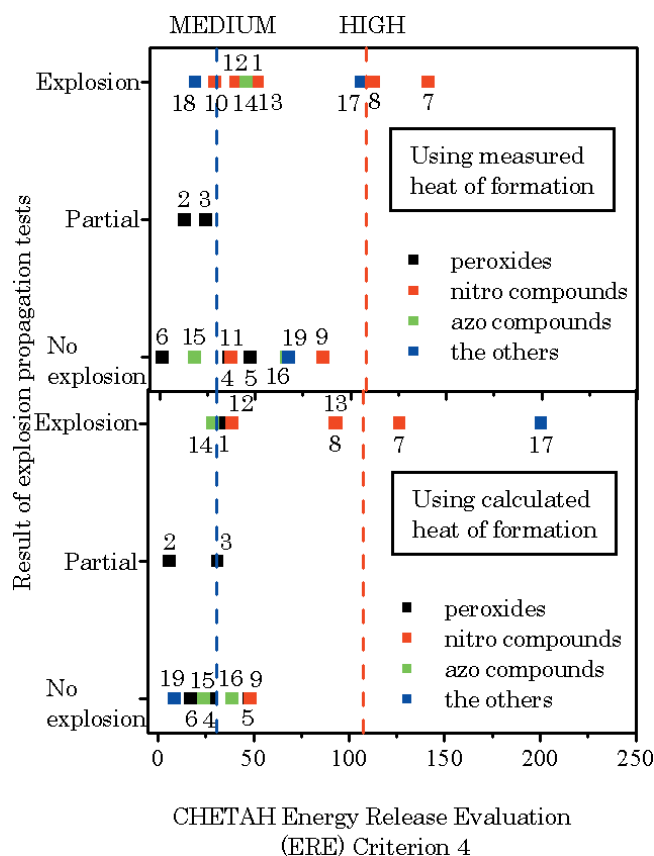


Fig. 4 The correlation of criterion 4 and literature data from explosion propagation tests.

atoms in the composition¹⁶. Figure 4 shows the correlation of criterion 4 and literature data from explosion propagation tests. Criterion 4 of two substances judged as “explosion” (10 and 18) by explosion propagation tests and two substances judged as “partial” (2 and 3) by explosion propagation tests were lower than 30, the “MEDIUM” rating threshold by CHETAH, when the measured heat of formation was used. Criterion 4 of one substance judged as “explosion” (14) by explosion propagation tests and one substance judged as “partial” (2) by explosion propagation tests was also lower than 30 when the calculated heat of formation by additivity rules was used. Since this criterion is evaluated utilizing criterion 1, this criterion ought to be closely related to criterion 1. When the orders according to the size of criteria 1 and 4 for each substance are compared, they are found to be similar. Therefore, criterion 4 is also a tentative criterion of the explosibility of self-reactive substances, but again, as in criterion 1, it is difficult to estimate the explosibility of substances by this criterion.

Criterion 5 is the “over-all energy release potential”. This criterion combines the above four individual criteria and the number of peroxide bonds into a single “HIGH” or “LOW” rating¹⁶. In this criterion, the weights assigned to the above four individual criteria were derived using a sophisticated pattern recognition technique with a large database of impact-tested materials^{16,27}. Namely, it is safe to say that this criterion is a semi-empirical one. Thus, it is likely that this criterion is an auxiliary indicator. Figure 5 shows the correlation of criterion 5 and literature data from explosion propagation tests. Two substances judged

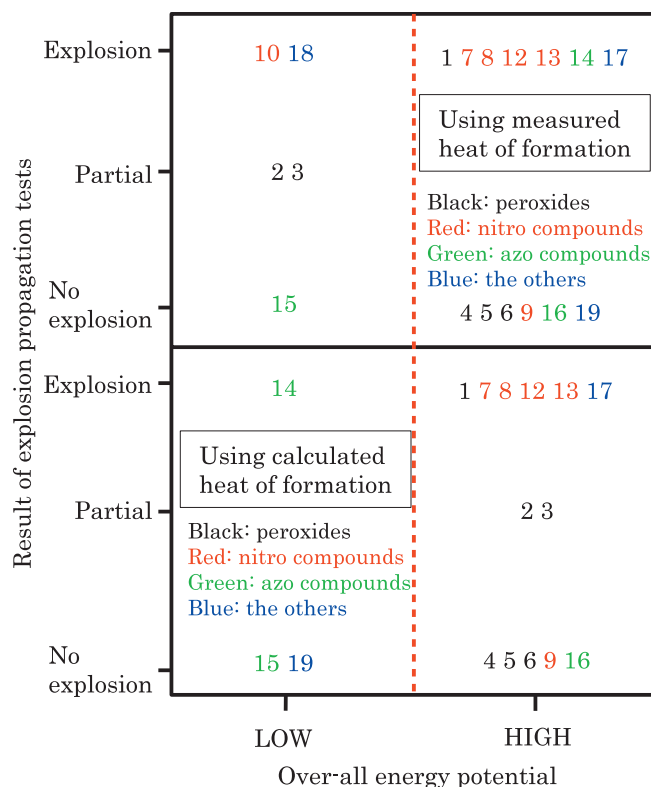


Fig. 5 The correlation of criterion 5 and literature data from explosion propagation tests.

as “explosion” (10 and 18) by explosion propagation tests and two substances judged as “partial” (2 and 3) by explosion propagation tests were rated “LOW” by CHETAH when the measured heats of formation were used. Similarly, in the case of calculated heats of formation by additivity rules, one substance judged as “explosion” (14) by explosion propagation tests was judged “LOW” by CHETAH. LPO (2), TBPB (3) (when using measured heat of formation), and AIBN (14) (when using calculated heat of formation), which were judged as “explosion” or “partial” by explosion propagation tests and rated “LOW” by criteria 2 and 3, were judged “LOW” by this criterion. This suggests that this criterion may not play an auxiliary role for the estimation of the explosibility of peroxides and azo compounds.

The explosibility of substances is known to be estimated by the combination of criteria 1 and 2²⁸. Figure 6 shows the correlation of criteria 1 and 2 of self-reactive substances when using measured heats of formation and heats of formation calculated by additivity rules. The red number indicates that the substance is judged as “explosion” by explosion propagation tests. The blue number indicates that the substance is judged as “partial” by explosion propagation tests. The green number indicates that the substance is judged as “no explosion” by explosion propagation tests. DNBA (8) was rated “HIGH” by CHETAH among substances judged as “explosion” or “partial” by explosion propagation tests. BPO (1), LPO (2), TBPB (3), and AIBN (14), judged as “explosion” or “partial” by explosion propagation tests, were rated “LOW” by CHETAH. Heats of decomposition of BPO (1), LPO (2), TBPB (3), and AIBN (14) are not very large and these

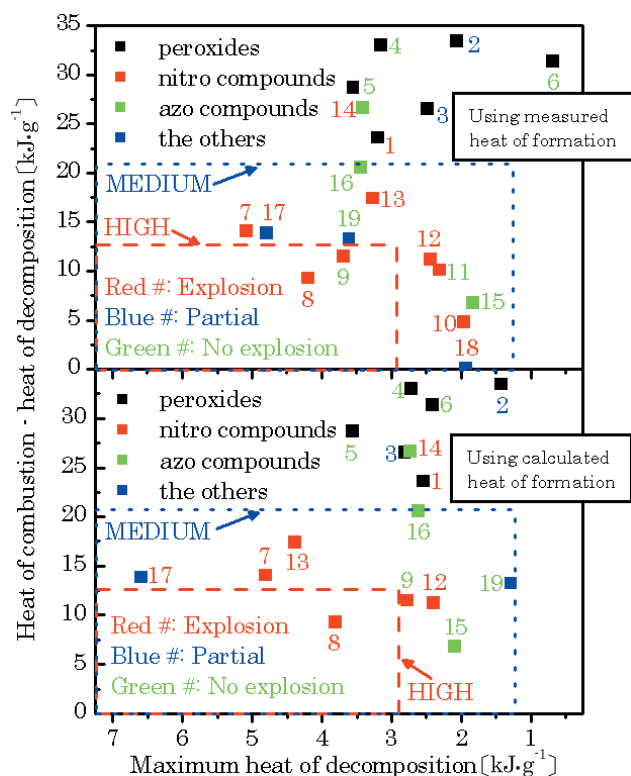


Fig. 6 The correlation of criteria 1 and 2 of self-reactive substances.

substances are evidently fuel-rich compositions. Therefore, the explosibility of organic peroxides and azo compounds, such as BPO and AIBN, may be assigned “LOW” rating by the estimation method of the combination of CHETAH criterion 1 and 2.

The accuracy of the heats of formation used for the calculation of CHETAH criteria was investigated. With respect to the group contributions to heat of formation in condensed states, Ijichi and Matsunaga compared the heats of formation estimated using the group contributions with literature data of heats of formation^(6),7). They proposed that the estimated heats of formation could be utilized to predict explosive hazards if the difference between the estimated heats of formation and literature data of heats of formation was less than 100 cal g⁻¹ (420 J g⁻¹)^(6),7). They argued that the difference in nitro compounds and organic peroxides was less than 420 J g⁻¹

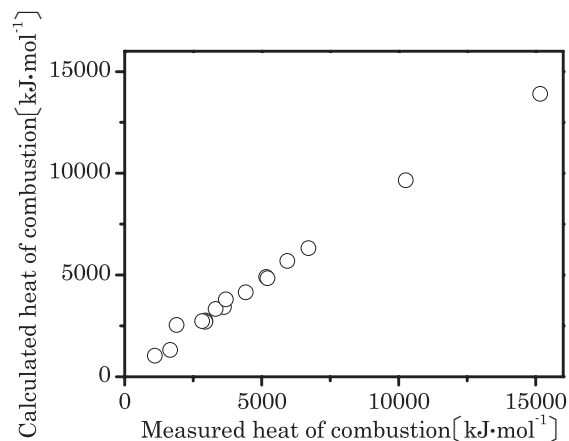


Fig. 7 The correlation of the measured heat of combustion and the calculated heat of combustion by CHETAH.

except in the case of propyl hydroperoxide^(6),7). Therefore it would be appropriate to utilize the group contributions for the prediction of explosibility. With respect to the measured heat of combustion, the relative error in measurement results was found to be less than 3%. It is reasonable to suppose that the relative error in heat of formation and heat of decomposition estimated by the measured heat of combustion will be approximately 3% based on the law of propagation of errors. It can be considered that there is little effect of the error size on the correlation between CHETAH criteria and the explosibility of substances. Moreover, Fig. 7 shows the correlation of the measured heat of combustion and the calculated heat of combustion by CHETAH. We see from Fig. 7 that there is a good correlation between the measured heat of combustion and the calculated heat of combustion.

3.2 Correlation of measurement data using ARC and the explosibility of self-reactive substances

Table 2 shows measurement results using ARC and literature data from explosion propagation tests. T_{ARC} is the onset temperature measured using ARC. T_p is the temperature at maximum pressure rising rate. Q_{ARC} is estimated assuming that the following heat balance is derived in an adiabatic system⁽²⁹⁾:

$$Q_{ARC} = \phi C_p (T_{max} - T_{ARC}), \text{ where } \phi \text{ is thermal inertia } (\phi$$

Table 2 Measurement results using ARC and literature data from explosion propagation tests.

Substances	Explosibility	The amount of samples for ARC [g]	T_{ARC} [°C]	T_p [°C]	Q_{ARC} [kJ · g ⁻¹]	P_{max} [kPa]	dP/dt_{max} [kPa · min ⁻¹]
BPO	+ (BAM)	0.0513	95	97	1.3	184	1.86
LPO	Partial (BAM)	1.0102	61	108	0.81	1002	5.04
TBPB	Partial (BAM)	0.3553	90	142	1.6	842	16.4
DPO	– (BAM)	0.6765	100	161	0.90	710	11.3
CHP	– (BAM)	0.3238	110	156	1.5	712	19.7
TBHP	– (BAM)	0.7496	85	152	1.1	2111	54.4
DNT	+ (BAM)	0.2232	235	280	3.7	1339	24.3
CNBA	+ (UN)	0.2678	276	304	1.3	1194	24.2
NPH	+ (UN)	0.6808	110	205	1.5	2308	140
AIBN	+ (BAM)	0.1519	87	90	1.2	382	6.18
ADCA	– (BAM)	0.1552	160	180	1.9	500	14.7

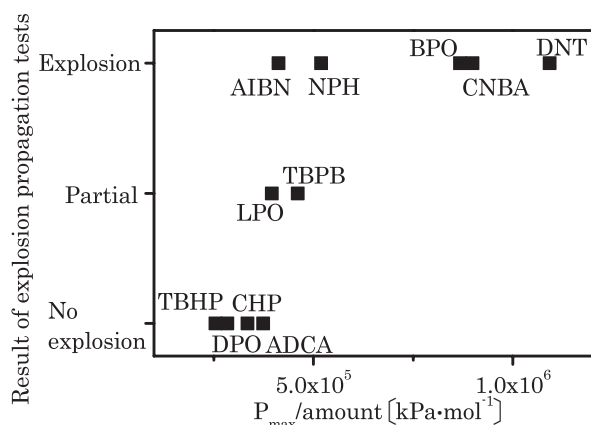


Fig. 8 The correlation of P_{\max} per unit mol of samples and literature data from explosion propagation tests.

value), C_p is the heat capacity of the sample (assumed to be $2.093 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1}$), and T_{\max} is the measured maximum temperature. P_{\max} is the measured maximum pressure, and dP/dt_{\max} is the measured maximum pressure rising rate.

DNT showed the largest Q_{ARC} . However, the Q_{ARC} did not correlate with the explosibility for other substances. Lu supposed that an exact heat of reaction could not be estimated using a Reactive System Screening Tool (RSST) apparatus because the change in heat capacity during the decomposition reaction was negligible when the heat of reaction of cumene hydroperoxide using RSST was investigated³⁰. RSST is designed to determine the potential for runaway reactions and to determine the temperature and pressure rise during a runaway reaction under quasi-adiabatic conditions. The energy release can be calculated in the same manner as ARC¹⁹. Moreover, Whitmore argued that energy release screenings were often overly conservative²⁰. Thus, the results of our experiment suggest an insufficient correlation between heat of decomposition using ARC and the explosibility of substances.

NPH showed the largest P_{\max} and dP/dt_{\max} . However, P_{\max} and dP/dt_{\max} were apparently not correlated with the explosibility for other substances. The amount of samples was determined such that the self-heating rate of the sample did not exceed the capacity of the heater on these ARC measurements. Since pressure under closed conditions is measured by ARC, the measured pressure is likely to be correlated with the amount of gaseous products in a sample vessel. Therefore, the pressure datapoints cannot be compared because the amount of samples is not equal. To compare the measured pressure data, P_{\max} and dP/dt_{\max} per unit amount of samples was calculated by division of the measurement data with the amount of samples and these data were compared with the explosibility of substances. Figure 8 shows the correlation of P_{\max} per unit mol of samples and literature data from explosion propagation tests. As shown, there is a good correlation between P_{\max} per unit mol of materials and the explosibility of substances. Using a statistical analysis, P_{\max} per unit mol of substances on the explosibility of substances has been shown to be

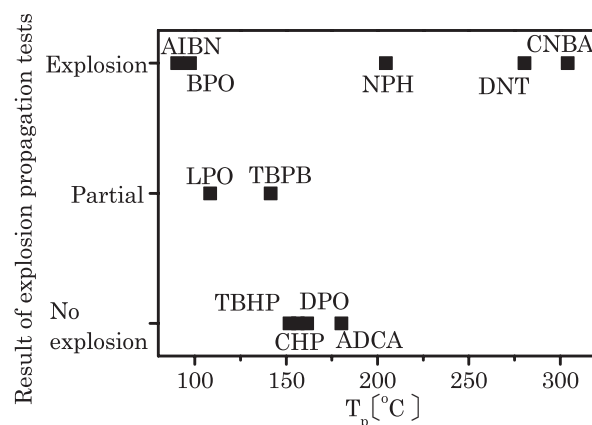


Fig. 9 The correlation of T_p and literature data from explosion propagation tests.

statistically significant at the 1% level.

However, P_{\max} per unit mol of AIBN (judged as “explosion” by explosion propagation tests), LPO (judged as “partial” by explosion propagation tests), and ADCA (judged as “no explosion” by explosion propagation tests) are not greatly different. Thus, the explosibility of substances could not always be estimated only by a maximum pressure per unit mol of materials. On the other hand, as shown in Fig. 9, the T_p of AIBN and LPO are 90 and 97°C, respectively, whereas the T_p of ADCA is considerably higher at 180°C. Consequently, it is probable that P_{\max} per unit mol of substances and T_p are correlated with the explosibility of substances. On the other hand, T_p of nitro compounds, NPH, DNT and CNBA, are not correlated with the explosibility of substances. It has been demonstrated in DSC analysis that onset temperatures of nitro compounds are higher than those of carboxylic acids which have little thermal hazards whereas those of organic peroxides are lower than those of carboxylic acid³¹. The fact that T_p of nitro compounds are higher than that of the other substances is similar to the above results in DSC analysis. In addition, BAM 50/60 steel tube test and UN gap test do not always give similar results. Thus, strictly speaking, it is desirable to correlate between measurement data using ARC and one of the two explosion propagation tests. However, even if the data of CNBA and NPH, which have been estimated by UN gap tests, is excluded, the above correlation is observed. Since P_{\max} per unit mol of substances and T_p are correlated with the explosibility of substances, the amount of gaseous products and the temperature at which the gases are generated by thermal decomposition are also likely to be correlated with the explosibility of substances. We are now examining the accuracy of the prediction by collecting more data. Moreover, strictly speaking, reactions at detonation or deflagration should be different from reactions at thermal decomposition. Thus, further theoretical investigations are necessary.

4. Conclusion

The correlation between estimated criteria using CHETAH and results of explosion propagation tests was investigated in order to evaluate the adequacy of

predicting the explosibility of substances using a thermochemical calculation technique. Moreover, correlations were made between measurement data using ARC and results of explosion propagation tests in order to evaluate the possibility of predicting the explosibility of substances by measuring values by ARC. The following conclusions can be drawn :

- (1) There is a mutual correlation between CHETAH criteria and the explosibility of self-reactive substances, except for organic peroxides and azo compounds.
- (2) There is a mutual correlation between the maximum pressure per unit mol of substances measured by ARC and the explosibility of substances. Additionally, the temperature at the maximum pressure rising rate is correlated with the explosibility of substances, except for nitro compounds. Therefore, the explosibility of self-reactive substances can be predicted by temperature and pressure measurements using ARC.

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熱量計および熱化学計算による 自己反応性物質の爆発性の予測

佐藤嘉彦^{*†}, 秋吉美也子^{*}, 三宅淳巳^{**}, 松永猛裕^{*}

自己反応性物質の爆発性を安全に予測することを目的として、CHETAHの計算結果およびARCの測定結果と、伝爆性試験（BAM 50/60鋼管試験もしくはUN gap試験）の結果を比較し、CHETAHの計算結果の妥当性の評価およびARC測定による爆発性予測の可能性の検討を行った。CHETAHによる爆発性の予測では、アゾ化合物や有機過酸化物を除いて爆発性を予測できた。一方、ARCによって測定された試料のモル単位の最大圧力と伝爆性試験の結果とは明らかな相関が見られた。また、ニトロ化合物を除いて、最大圧力上昇速度を示す温度と伝爆性試験の結果には相関があった。これらの結果により、自己反応性物質の爆発性の予測にARCによる圧力測定が有用である可能性が示された。

^{*}独立行政法人産業技術総合研究所安全科学研究部門爆発安全研究コア

〒305-8565 茨城県つくば市東1-1-1 中央第5

TEL : 029-861-4785

[†]Corresponding address : yoshihiko-satou@aist.go.jp

^{**}横浜国立大学大学院環境情報学府

〒240-8501 横浜市保土ヶ谷区常盤台79-7