REITP3 - Hazard evaluation program for heat release based on thermochemical calculation

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REITP3 - A hazard evaluation program for heat release based on thermochemical calculation has been developed by modifying REITP2 (Revised Estimation of Incompatibility from Thermochemical Properties[2]). The main modifications are as follows.

(1) Reactants are retrieved from the database by chemical formula.
(2) As products are listed in an external file, the addition of products and change in order of production can be easily conducted.
(3) Part of the program has been changed by considering its use on a personal computer or workstation.

These modifications will promote the usefulness of the program for energy hazard evaluation.

1. Introduction

In order to estimate the energy release behavior of energetic materials, the heat of reaction is an essential property and several methods are devised to do it[1,2]. By using REITP2 (Revised Estimation of Incompatibility from Thermochemical Properties[2,3], from the molecular formula and heat of formation of the reactants, heats of reaction are calculated by assuming the products. The relationship between the heat of reactions calculated by REITP2 and the experimental results such as explosion heats and ballistic mortar values has been demonstrated[3,4].

REITP2 is intended to be used on a mainframe computer with Fortran. However, based on the downsizing and highly developed performance of computers, it should work on a personal computer or workstation. Several revisions of the program are also expected. Therefore, we have devised the computer program REITP3 by making some modifications to the REITP2 program. The main changes are shown and examples of the calculation are demonstrated.

2. Modification of the program

We have made several changes to the inputs and

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other modifications, while the principle of the calculation is the same. The main modifications are as follows.

(1) Reactants are retrieved from the database by chemical formula.
Index numbers were used in REITP2, but chemical formula inputs are more facile and added to the input option.

(2) As products are made to be listed in an external file, the addition of products and change of production order can easily be conducted.
Incorporation of the products inside the program as data statements limited the usefulness of REITP2. Therefore, reading products from an external file is fulfilled. A part of the product file is shown in Fig. 1. Chemical formulas and heats of formation are listed in it. The order is based on the heat of formation per weight[4]. If new products are assumed, the addition of data to the product file enables it. If the order of production is changed, the order can be renumbered.

(3) Part of the program has been modified by considering the use on a personal computer or workstation.
File declarations for reactants file (date bank), etc. have been changed.

The operation of the program compiled with Lahey[5] Fortran77 has been confirmed on a personal computer with Pentium processor operated by Microsoft Windows 95.

The operation in workstation with Fortran77 compiler has been confirmed on Fujitsu S-4/20 with SunOS. Also it has been confirmed on HITACHI MP5800/320 with HI-OSF/1-MJ(UNIX).

Calculation examples are demonstrated in Figs. 2 and 3. This is the estimation of the heat of reaction of the mixture of 1H-tetrazole and sodium nitrate. Calculations were conducted by the input of a chemical formula as shown in Fig. 2. When the assumption of the products was changed, that is, NaOH was excluded from the products, the result changed as shown in Fig. 3.

Besides the above modifications, some changes have been made, such as increased compounds in the reactant file. Heats of formation, especially for organic compounds, can be estimated by the group additivity method or several other methods[6-10]; therefore, REITP3 can be a useful tool to estimate the heats of reaction and decomposition for energetic materials.

3. Conclusions

REITP3 - A Hazard evaluation program for heat release based on thermochemical calculations has been developed by modifying REITP2. It works on personal computers and workstations and inputs have become more facile. It is expected that these modifications of the REITP program will promote its usefulness for the evaluation of energy release hazard.

BeO	Be	1O	1O	0	146.0
LiF	Li	1F	1F	0	146.3
Be(OH)2	Be	1O	2H	2	216.5
BeF2	Be	1F	2F	0	227.0
Li2O	Li	2O	1O	0	142.5
Be2SiO4	Be	2Si	1O	4	513.7
Al6Si2O3	Al	6Si	2O	3	1903.0
B2O3	B	2O	3O	0	302.0
MgF2	Mg	1F	2F	0	263.5
BF3	B	1F	3F	0	265.4
Al(OH)3	Al	1O	3H	3	305.0
H2O(l)	H	2O	1O	0	68.3
Mg(OH)2	Mg	1O	2H	2	221.0
Al2O3	Al	2O	3O	0	384.8
CaF2	Ca	1F	2F	0	290.3
AlF3	Al	1F	3F	0	311.0
Mg2SiO4	Mg	2Si	1O	4	519.6
MgO	Mg	1O	1O	0	143.8
SiF4	Si	1F	4F	0	370.0
BeCO3	Be	1C	1O	3	245.0
(BOH)3	B	3O	3H	3	289.0
Na2SiO3	Na	2Si	1O	3	371.6
K2SiO3	K	2Si	1O	3	370.0
SiO2	Si	1O	2O	0	205.4
NaF	Na	1F	1F	0	136.0
NaOH	Na	1O	1H	1	101.7
H2O(g)	H	2O	1O	0	57.8
HF	H	1F	1F	0	64.2
Sc2O3	Sc	2O	3O	0	410.0
BeCO3	Be	1C	1O	3	288.5
BeSO4	Be	1S	1O	4	288.1
TiO2	Ti	1O	2O	0	218.0
CaO	Ca	1O	1O	0	151.9

Fig.1 Example of the data contained in product file for REITP3.

```
% REITP3
Now, reading data. Just a moment, please.

Input the option number like 11131.
Instruction, input 80000.
Search the Index Number, input 70000.
End this program, input 90000.
[ ]

80000
Explanation of the Option Numbers
OPTKIN=0 Decomposition of Single Compound
         1 Reaction of Two Materials
         2 Reaction of Materials (Fixed Ratios)
         3 Calculation of Cabinet or Room
OPTH2O=0 Produced Water will be assumed as Liquid
         1 Produced Water will be assumed as Gas
OPTINP =0 All Data input
         1 Index Number input
         2 Molecular Formula input
OPTOUT=0 Minimum output
         1 Medium output
         2 Maximum output
         3 Diagram output(OPTKIN=1 or 2)
OPTCOR=0 No correction
         1 Values corrected with Oxygen Balance
         2 Values assumed as CO2 would be produced after CO

Input the option number like 11131.
Instruction, input 80000.
Search the Index Number, input 70000.
End this program, input 90000.
[ ]

11220

 OPTKIN = 1  OPTH2O = 1  OPTINP = 2  OPTOUT = 2  OPTCOR = 0

Reaction of Two Compounds (Optimization)

[   Title

Example
Example
[   Header

1H-tetrazole + Sodium nitrate
1H-tetrazole + Sodium nitrate


Return to Menu,   input "END" or "E"
Stop this program, input "STOP" or "S"
Put out a Table,  input "TABLE" or "T"
[Molecular Formula]

C1H2N4
   C1H2N4          =C  1H  2N  4
  1    1H-TETRAZOLE          HF=  56.64   INDEX=5100001
Return to Menu,   input "END" or "E"
Stop this program, input "STOP" or "S"
Put out a Table,  input "TABLE" or "T"
[Molecular Formula]
```

```
NaIN1O3
NaIN1O3          = Na 1 N 1 O 3
1   SODIUM NITRATE          HF=-111.54   INDEX=1040030
NaIN1O3          = Na 1 N 1 O 3
Put out to Printer[P], File[F], or Not[N] ?
#
N

########## Reaction of Two Materials ##########################################

1H-TETRAZOLE      C H N                              56.64 5100001
                  1 2 4
        Molecular Weight of Compound  =  70.05
        Oxygen Balance of Compound    = -68.52

SODIUM NITRATE    Na N O                            -111.54 1040030
                  1 1 3
        Molecular Weight of Compound  =  84.99
        Oxygen Balance of Compound    =  47.06

*** Products ***************************************************************
    Name of Products      Amount (mol)      Heat of Formation (kcal/mol)

    NaOH                    0.2887                -101.70
    H2O(g)                  0.5669                 -57.80
    CO2                     0.0053                 -94.10

*** Remained Elements ******************************************************

    Name of Atoms         Amount (mol)

    C                       0.7060
    N                       3.1338

******************************************************************************

                          wt. percent     mol. ratio     mol. percent
    1H-TETRAZOLE              67             1.00            71
    SODIUM NITRATE            33             0.41            29

    Oxygen Balance of Mixture = -30.38

******************************************************************************

    The Maximum Heat of the Reaction =    -71   (kcal/mol of Reactants)

                                     =    -950  (cal/gram of Reactants)

    The Grade of Danger  = A

******************************************************************************

    Return to Menu,   input "END" or "E"
    Stop this program, input "STOP" or "S"
    Put out a Table,  input "TABLE" or "T"
    [Molecular Formula]

    S
    %
```

Fig.2 Example of REITP3 calculation for the heat of reaction of two materials (Inputs from the keyboard are underlined.)

*** Products **********

Name of Products	Amount (mol)	Heat of Formation (kcal/mol)
H2O(g)	0.4574	-57.80
Na2CO3	0.2713	-270.40
CO2	0.1782	-94.10

*** Remained Elements **********

Name of Atoms	Amount (mol)
C	0.0080
N	2.3723

****

	wt. percent	mol. ratio	mol. percent
1H-TETRAZOLE	41	1.00	46
SODIUM NITRATE	59	1.19	54

Oxygen Balance of Mixture = -0.33

****

The Maximum Heat of the Reaction = -82 (kcal/mol of Reactants)

= -1050 (cal/gram of Reactants)

The Grade of Danger = A

****

Fig.3 Calculation result for the heat of reaction of 1H-tetrazole and $NaNO_3$ when NaOH was excluded from product file

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熱化学計算による熱放出危険性評価プログラムREITP3

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潜在的混触発火危険性評価プログラムREITP2を改良し、熱放出危険性評価プログラムREITP3を作成した。主な改良点は、(1)化学式によりデータベース中の反応物を呼び出せること、(2)生成物データを外部ファイルとしたので、生成物の追加、生成順位の変更が容易になったこと、(3)パーソナルコンピュータやワークステーションでの使用を考慮してプログラムを変更したことなどである。このプログラムが、エネルギー放出危険の評価に、一層役立つものと考えられる。

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