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An Insensitive Booster Explosive: DAAF Surface-coated with Viton A

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1 Thermal decomposition analysis

1.1 Non-isothermal kinetics analysis

The equations for Kissinger's method, Ozawa's method and Starink's method are as follows:

$$\ln\left(\beta/T^{s}\right)=-\left(BE/RT\right)+C \tag{1}$$

where T is the peak temperature in K, E is the apparent activation energy in kJ·mol^{-1}, R is the gas constant (8.314 J·K^{-1}·mol^{-1}), β is the linear heating rate in K·min^{-1}, and B and C are constants. When $s = 2$ and $B = 1$, Equation (1) is according to Kissinger's method. When $s = 0$ and $B = 1.0516$, Equation (1) is according to Ozawa's method. When $s = 1.8$ and $B = 1.0037$, Equation (1) is according to Starink's method. Based on the exothermic peak temperature measured at four different heating rates, 5, 10, 15 and 20 °C·min^{-1}, the three methods were applied to study the kinetic parameters of the title compound. From the original data, the apparent activation energy E, pre–exponential factor A, linear coefficient R and standard deviation S were determined based on the relationships of $\ln(\beta/T^{2})$, $\ln(\beta/T^{1.8})$ and $\ln\beta$ to $1/T$, corresponding to Kissinger's method, Starink's method, and Ozawa's method, respectively.

1.2 Calculation of the critical temperature of a thermal explosion, ΔS≠, ΔH≠ and ΔG≠

The value of the peak temperature corresponding to $\beta \rightarrow 0$ (T_0), the corresponding critical temperature of thermal explosion (T_b), entropy of activation ($\Delta S^{\neq}$), enthalpy of activation ($\Delta H^{\neq}$), and free energy of activation ($\Delta G^{\neq}$) were obtained by the following Equations (2), where a, b and c are coefficients, k_B is Boltzmann's constant (1.381×10^{-23} J/K) and h is Planck's constant (6.626×10^{-34} J·s).

$$T_i = T_0 + a\beta + b\beta^2$$

$$T_b = \left(E - \sqrt{E^2 - 4ERT_0}\right)/2R$$

$$A = \left(k_B T_0/h\right)\exp\left(1 + \Delta S^{\neq}/R\right)$$

$$\Delta H^{\neq} = E - RT_0$$

$$\Delta G^{\neq} = \Delta H^{\neq} - T_0 \Delta S^{\neq} \tag{2}$$

2 Detonation Velocity

In the detonation characteristics of explosives, detonation velocity is an essential indicator. Many empirical and semi-empirical formulas for estimating the detonation velocity have been accumulated and summarized. One of the most widely used is the Urizar method. The principle is that the detonation velocity of a mixed explosive is equal to the volume fraction of each component multiplied by the sum of the detonation velocity of each component. The specific method is described in Equations (3):

$$V_D = \sum (V_{Di} W_{vi})$$

$$\rho_T = \sum \mathrm{m_i} / \sum V_\mathrm{i}$$

$$V_T = \sum \frac{m_i}{\rho_{Ti}}$$

$$V = V_\mathrm{T}/0.95$$

$$w_\mathrm{i} = v_\mathrm{i}/v \tag{3}$$

V_{Di} is the detonation velocity of ingredient i in m·s^{-1}, W_{vi} is the volume fraction of that ingredient v_i, ρ_T is the theoretical density of the mixed explosive in g·cm^3, ρ_{Ti} is the detonation density of ingredient i. m_i is the quantity of ingredient i. V_i is volume of ingredient i in cm^3. V_T is the theoretical volume of the mixed explosive in cm^3, V is the actual volume of the mixed explosive in cm^3. w_i is the volume fraction of the ingredient i. By investigating "Military Explosives" the data is listed in the Table S1.

Table S1. Parameters of a three component explosive

Components	Detonation velocity [m/s]	Density [g/cm^3]
DAAF	8020	1.747
TATB	7963	1.938
HMX	9122	1.91

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