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Hydrazine 5, 5′-Bitetrazole-1, 1′-diolate: A Promising High Density Energetic Salt with Good Properties

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Supporting Information

Experimental

Measurements

Elemental analyses were performed on a Flash EA 1112 full-automatic trace element analyzer. The FT-IR spectra were recorded on a Nexus-470 FT-IR (Nicolet) spectrometer (KBr pellets) in the range of 4000 - 400 cm^{-1} with a resolution of 6 cm^{-1}. ^{1}H and ^{13}C NMR spectra were obtained using a JEOLJNM-ECA400 at 400 MHz. The morphologies of the salt was examined with a HITACHI (Japan) S-3400N-II Scanning Electron Microscope (SEM) at 5 kV and 10 mA. Differential scanning calorimeter (DSC) and thermal gravity analysis - differential thermal gravity analysis (TG-DTG) measurements were carried out by using Pyris-1 differential scanning calorimeter and Pyris-1 thermogravimetric analyzer (Perkin Elmer, USA) under dry nitrogen atmosphere with flowing rate of 20 mL min^{-1}, samples about of 0.1 mg were placed in aluminum pans with various heating rates of (5, 10, 15, and 20) °C min^{-1}. The constant-volume energy of combustion were measured by a Parr-6200 bomb calorimeter (Parr, USA). Impact sensitivity was determined by Fall Hammer Method using BAM FALL HAMMER BFH-10, and frication sensitivity was determined with a BAM FRICTION APPARATUS FSKM -10 by using BAM standards.

Crystallographic data collection and refinement

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Table S1 Hydrogen bond lengths (Å) and bond angles (°) for HA·BTO

D-H···A	*d*(D-H)	*d*(H···A)	*d*(D···A)	angle(D-H···A)	Symmetry code
298K					
N5-H5A···O1	0.890	1.796	2.673	168.31	x+1, y, z
N5-H5A···N1	0.890	2.503	3.300	149.40	x+1, y, z
N5-H5A···N2	0.890	2.636	3.169	119.34	x+1, y, z
N5-H5B···O1	0.890	1.873	2.743	165.31	
N5-H5C···N3	0.890	2.065	2.835	144.12	x+1, y, z+1
N5-H5C···N2	0.890	2.639	3.231	124.83	-x+1, -y+2, -z+1
153K					
N5-H5C···N3	0.840	2.050	2.827	153.00	-x+1, -y+1, -z+3
N5-H5B···O1	0.840	1.920	2.743	166.00	-x, -y+1, -z+2
N5-H5C···O1	0.840	1.860	2.684	168.00	-x+1, -y+1, -z+2
N5-H5C···N2	0.840	2.620	3.167	124.00	-x+1, -y+1, -z+2
N5-H5A···N1	0.840	2.530	3.307	154.00	-x+1, -y+1, -z+2

Results and discussion

Thermal analysis

The equations of the Kissinger's and Ozawa-Doyle's methods are as follows (T_p is the peak temperature, °C; R is the gas constant, 8.314 J mol^{-1} K^{-1}; β is the linear heating rate, °C min^{-1} and C is a constant):

$$\ln(\frac{\beta}{T_p^2}) = \ln(\frac{A_k R}{E_k}) - \frac{E_k}{R}\frac{1}{T_p} \quad \text{(S1)}$$

$$\log\beta + \frac{0.4567E_o}{RT_p} = C \quad \text{(S2)}$$

The thermal explosion critical temperature (T_{bp}) is calculated by using the method in equations (S3) and (S4), according to literatures [36, 37]. The value of the peak temperature (T_{p0}) for the salt is obtained as 232.1 °C, corresponding to $\beta \rightarrow 0$, where a, b and c are coefficients.

$$T_{pi} = T_{p0} + a\beta + b\beta^2 + c\beta^3 \quad \text{(S3)}$$

The corresponding critical temperature of thermal explosion (T_b) is then obtained by equation (4).

$$T_{\mathrm{bp}}=\frac{E-\sqrt{E^2-4ERT_{\mathrm{p0}}}}{2R} \tag{S4}$$

The entropies activation ($\Delta S^{\neq}$), enthalpies activation ($\Delta H^{\neq}$), and free energies of activation ($\Delta G^{\neq}$) of the decomposition reaction of the salt HA·BTO are obtained by the following equations (S5)-(S7) according to literatures [38,39], in which k_B is the Boltzmann constant (1.381×10^{-23} J K^{-1}) and h is the Planck constant (6.626×10^{-34} J s).

$$A=\frac{k_{\mathrm{B}}T}{h}\mathrm{e}^{\Delta S^{\neq}/R} \tag{S5}$$

$$\Delta H^{\neq}=E-RT \tag{S6}$$

$$\Delta G^{\neq}=\Delta H^{\neq}-T\Delta S^{\neq} \tag{S7}$$

Energetic Properties

The detonation parameters of HA·BTO including the detonation velocity (D), pressure (P) are predicted by Empirical Kamlet-Jacobs equations [41]:

$$D=1.01(NM^{0.5}Q^{0.5})^{0.5}(1+1.30\rho) \tag{S8}$$

$$P=1.558\rho^2NM^{0.5}Q^{0.5} \tag{S9}$$

Where D is the detonation velocity (m s^{-1}); P is the detonation pressure (GPa); N is the moles of detonation gases per gram explosive; M is the average molecular weight of these gases; Q is the energy of explosion (kJ kg^{-1}); ρ is the loaded density of explosives (g cm^{-3}).