Synthesis, Structure and Energetic Properties of a Catenated N_6, Polynitro Compound: 1,1'-Azobis(3,5-dinitropyrazole)

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Abstract: A nitrogen-rich, polynitro energetic compound with an N,N-azo linkage, 1,1'-azobis(3,5-dinitropyrazole) (ABDNP), has been synthesized by an oxidative coupling reaction of 1-amino-3,5-dinitropyrazole with different oxidizing agents. The target compound was characterized by IR spectroscopy, ^1H and ^{13}C nuclear magnetic resonance spectroscopy, elemental analysis, mass spectra, X-ray diffraction and differential scanning calorimetry (DSC). The DSC results show that 1,1'-azobis(3,5-dinitropyrazole) decomposes at a relatively high onset temperature (202.9 °C), which indicates that 1,1'-azobis(3,5-dinitropyrazole) has acceptable thermal stability. The energetic properties were obtained, with a measured density and heat of formation matched by theoretically computed values based on the B3LYP method.

Keywords: energetic compound, 1,1'-azobis(3,5-dinitropyrazole), synthesis, energetic properties

1 Introduction

Traditional energetic materials, including quintessential explosives such as HMX (1,3,5,7-tetranitro-1,3,5,7-tetrazocane), RDX (1,3,5-trinitro-1,3,5-triazinane) and TNT (2,4,6-trinitrotoluene), are based on the oldest design strategy of energetic materials: the presence of fuel and oxidizer in the same molecule.

New strategies in energetic materials' research focus on nitrogen-rich/high positive heat of formation compounds [1-5]. Nitrogen-rich compounds have therefore received increasing attention as promising candidates for high energy-density materials (HEDM), which might be used as propellants, explosives or especially as gas generators [6-9]. The generation of nitrogen gas as an end product from nitrogen-rich compounds is highly desirable for the enhancement of energy and avoidance of environmental pollution [10-13]. Nitrogen-rich compounds based on C/N heteroaromatic rings with high nitrogen content, such as triazole, tetrazole, triazine and tetrazine, are at the forefront of high energy research [14, 15]. Recently, the combination of an azo group with nitrogen-rich heteroaromatic rings has been extensively studied because the azo linkage not only desensitizes but also dramatically increases the heat of formation of high-nitrogen compounds such as 3,3'-azobis(1,2,4-triazole) (1) [16], 5,5'-dinitro-3,3'-azo-1H-1,2,4-triazole (2) [17], 3,3'-azobis-(6-amino-1,2,4,5-tetrazine) (3) [18], 4,4',6,6'-tetra(azido)azo- 1,3,5-triazine (4) [19], these being four representative compounds of this type (Scheme 1), where the two heteroaromatic rings are connected by a C−N=N−C linkage. However, if the azo group were attached to the nitrogen of the heteroaromatic rings to create a rather long chain of catenated nitrogens (N−N=N−N linkage), such a polynitrogen structure could result in energetic compounds with unique properties and features.

In the pursuit of novel nitrogen-rich energetic materials, some catenated nitrogen compounds containing the N−N=N−N linkage have been synthesized in recent years, such as 4,4'-azo-1,2,4-triazole (5) [16, 20, 21], 1,1'-azobis-1,2,3-triazole (6) [22], 1,1'-azobis(tetrazole) (7) [23], 2,2'-azobis(5-nitrotetrazole) (8) [24] and 1,1'-azobis(5-methyltetrazole) (9) [25] (Scheme 2). Unfortunately, most of the above compounds do not exhibit excellent detonation performance (such as compounds 5, 6, 9) or thermal stability (such as compounds 7, 8, 9).

By comparison with the above catenated nitrogen energetic materials, 1,1'-azobis(3,5-dinitropyrazole) (ABDNP, 10) was found to exhibit relatively good density, detonation energy and thermal stability, its synthesis being reported by our research group in a short communication [26]. In the present paper, we report that treatment of an acetonitrile solution of 1-amino-3,5-dinitropyrazole (ADNP) with tert-butyl hypochlorite (t-BuOCl), sodium dichloroisocyanurate (SDCI) or trichloroisocyanuricacid (TCICA) leads to the formation of ABDNP (Scheme 3) as a yellow solid. The structure of ABDNP was fully characterized by ^{1}H and ^{13}C NMR spectroscopy, IR spectroscopy and elemental analysis. The single crystal structure of ABDNP·2DMSO was determined by X-ray diffraction. The energetic properties of ABDNP were also investigated.
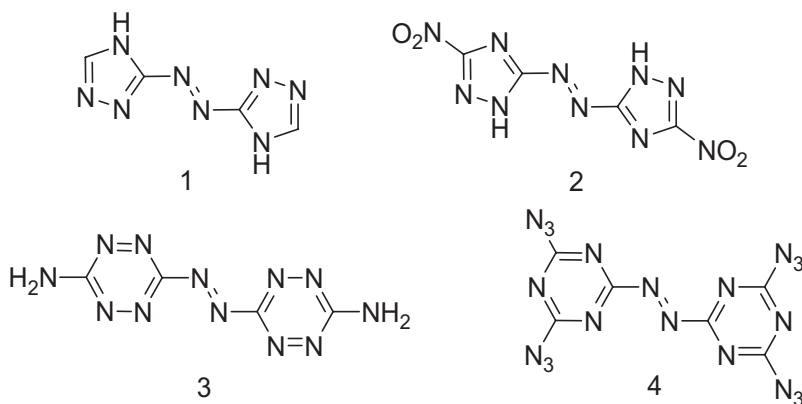
Scheme 1. Examples of reported high-nitrogen compounds with C,C'-azo linkages
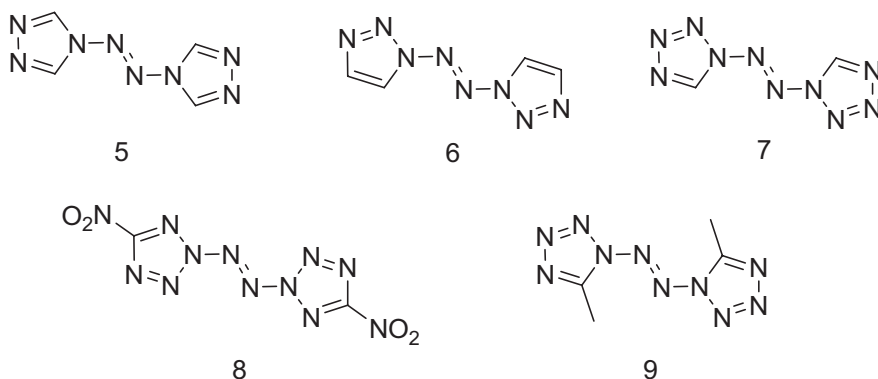
Scheme 2. Examples of reported high-nitrogen compounds with N,N'-azo linkages
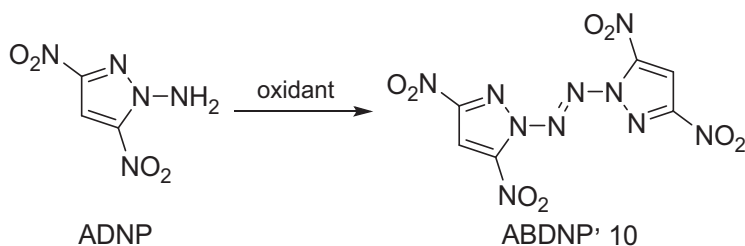
Scheme 3. Azo coupling reaction of 1-amino-3,5-dinitropyrazole with different oxidants

2   Experimental

Caution: Although we experienced no problems during the synthesis of the reported compounds, standard safety precautions (leather gloves, face shield and ear plugs) should be used when handling this energetic material.

2.1 General methods

ADNP was synthesized in house, but other reagents (of analytical grade) were obtained from commercial suppliers and used without further purification. Infrared (IR) spectra were recorded utilizing a NEXUS 870-based Fourier transform infrared spectrometer employing a KBr matrix. ^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra were recorded on a Bruker AV 500 NMR spectrometer with TMS as the internal standard. Mass spectra were acquired using a GCMS-QP 2010 Micromass UK spectrometer. Elemental analysis was performed using a Vario EL-III Elemental Analyzer. DSC was performed in a platinum sample container using a Shimadzu DSC-60 instrument, the 0.5-1.0 mg sample being heated at a rate of 5 °C·min^{-1}.

2.2 X-Ray crystallography

A crystal of compound ABDNP·2DMSO suitable for X-ray crystallographic analysis was obtained by slow evaporation of a DMSO solution of compound 10. The single crystal structure was determined using a Bruker SMART APEXII CCD X-ray diffractometer equipped with graphite-monochromatized Mo Kα radiation (0.71073 Å) and the SHELXTL crystallographic software package. Data were collected by the ω scan technique. The structure was solved by direct methods using SHELXS-97 and expanded using the Fourier technique. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were determined by theoretical calculations and refined using an isotropic vibration factor.

2.3 Synthesis of *O*-mesitylenesulfonylhydroxylamine (MSH)

Mesitylenesulfonyl chloride (24.0 g, 0.11 mol) was added with stirring to a solution of ethyl acetohydroxamate (11.3 g, 0.11 mol) and triethylamine (11.0 g, 0.11 mol) in dimethylformamide (41.0 mL) cooled in ice-water. After 1 h at 15 °C, the reaction mixture was poured into ice-water, the precipitate was filtered off, washed with water and dried to give *O*-mesitylenesulfonylacetohydroxamate (EMSAH) as a white solid in 95.6% yield (31.0 g). ^{1}H NMR (CDCl$_3$, 500 MHz), δ: 1.173-1.202 (t, 3H, J = 14.5 Hz), 2.041 (s, 3H), 2.314 (s, 3H), 2.646 (s, 6H), 3.888-3.931 (t, 2H, J = 21.5 Hz), 6.969 (s, 2H); ^{13}C NMR (CDCl$_3$, 125 MHz), δ: 13.98, 14.87, 21.07, 22.83, 63.61, 130.39, 131.52, 140.71, 143.32, 169.24;

IR (KBr, cm^{-1}), υ: 2981, 2941 (−CH$_2$, −CH$_3$), 787, 669 (benzene ring), 1636 (C=N). Anal. calcd. for C$_{13}$H$_{19}$NO$_4$S: C 54.72%, H 6.71%, N 4.91%; found C 54.63%, H 6.82%, N 4.98%.

EMSAH (10.0 g, 0.035 mol) was dissolved in 1,4-dioxane (20.0 mL) at room temperature, and 70% perchloric acid (12.0 mL) was added dropwise at 0-5 °C. The solution was poured into ice-water after stirring at 0-5 °C for a further 0.5 h, extracted with dichloromethane (3 × 60.0 mL), dried with magnesium sulfate, and the dichloromethane was evaporated under reduced pressure to give *O*-mesitylenesulfonylhydroxylamine (MSH) as a white solid in 74.3% yield (5.6 g), m. p.: 79.3 °C (DSC, decomposition). ^{1}H NMR (DMSO-d$_6$, 500 MHz), δ: 2.177 (s, 3H), 2.506 (s, 6H), 6.773 (s, 2H), 9.242 (s, 2H); ^{13}C NMR (DMSO-d$_6$, 125 MHz), δ: 20.76, 23.18, 130.45, 136.42, 137.14, 142.63; IR (KBr, cm^{-1}), υ: 3340, 3270 (−NH$_2$), 3035 (benzene-H), 2987, 2945 (−CH$_3$), 779, 689 (benzene ring). Anal. calcd. for C$_9$H$_{13}$NO$_3$S: C 50.21%, H 6.09%, N 6.51%; found C 50%.33, H 6.15%, N 6.44%.

2.4 Synthesis of 1-amino-3,5-dinitropyrazole (ADNP)

3,5-Dinitropyrazole (2.0 g, 12.7 mmol) was dissolved in ethanol (15.0 mL) at room temperature, and a 5% ethanolic solution of potassium hydroxide (14.2 mL, 0.71 g, 12.7 mmol) was added dropwise at 5-10 °C. After 2 h at room temperature, the precipitate was filtered off, washed with ethanol and ice-water, and dried to give the potassium salt of 3,5-dinitropyrazole (DNPK) as a yellow solid in 90.7% yield (2.25 g). ^{1}H NMR (D$_2$O-d$_2$, 500 MHz), δ: 7.399 (s, 1H, −CH); ^{13}C NMR (D$_2$O-d$_2$, 125 MHz), δ: 99.24, 156.18; IR (KBr, cm^{-1}), υ: 3157 (−CH), 1539, 1378, 1351 (−NO$_2$), 1270, 835, 755 (pyrazole). Anal. calcd. for C$_3$HN$_4$O$_4$K: C 18.37%, H 0.51%, N 28.56%; found C 18.40%, H 0.49%, N 28.54%.

DNPK (0.5 g, 2.55 mmol) was dissolved in anhydrous acetonitrile (15.0 mL) at room temperature. A solution of MSH (0.77 g, 3.57 mmol) in anhydrous acetonitrile (2.5 mL) was added dropwise to the DNPK solution at 0-3 °C. After 20 h at room temperature, the precipitate was filtered off, and the filtrate was concentrated *in vacuo* to give a yellow oil. Recrystallization from water gave a buff solid, 1-amino-3,5-dinitropyrazole (ADNP) in 84.1% yield (0.37 g), m. p.: 111.3-112.0 °C. ^{1}H NMR (DMSO-d_6, 500 MHz), δ: 7.105 (s, H, −CH), 8.006 (s, 2H, −NH$_2$); ^{13}C NMR (DMSO-d_6, 125 MHz), δ: 101.69, 140.07, 147.66; IR (KBr, cm^{-1}), υ: 3355, 3287 (−NH$_2$), 3154 (−CH), 1508, 1381, 1356 (−NO$_2$), 1556, 845, 741 (pyrazole). Anal. calcd. for C$_3$H$_3$N$_5$O$_4$: C 20.82%, H 1.75%, N 40.46%; found C 20.80%, H 1.78%, N 40.50%.

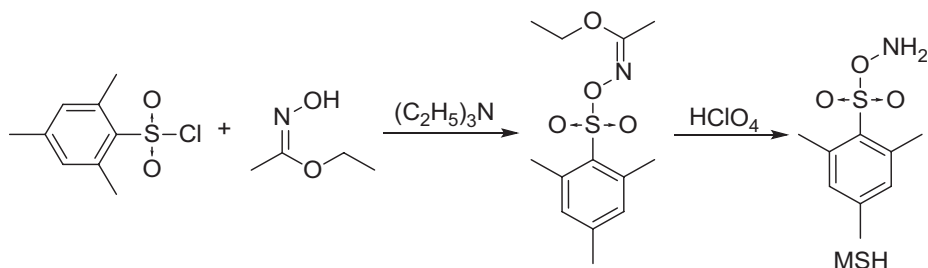## 2.5 Synthesis of 1,1'-azobis(3,5-dinitropyrazole) (ABDNP)

1-Amino-3,5-dinitropyrazole (0.1 g, 0.58 mmol) was dissolved in acetonitrile (10.0 mL) at room temperature, cooled to 0-5 °C with stirring under nitrogen and treated with t-butyl hypochlorite (0.082 g, 0.75 mmol) during 3 min. The resulting solution was stirred at 20-25 °C for a further 2 h, concentrated *in vacuo*, and triturated with isopropyl alcohol (2.0 mL). The precipitate was filtered off, washed with isopropyl alcohol and ice-water, and dried to give a yellow solid in 43.5% yield (43.0 mg). ^{1}H NMR (DMSO-d_6, 500 MHz), δ: 8.625 (s, 2H, 2CH); ^{13}C NMR (DMSO-d_6, 125 MHz), δ: 106.03, 146.09, 153.39; ^{14}N NMR (DMSO-d_6, 58 MHz), δ: −124.15, −68.56, −32.80, −23.21, −3.260; ^{15}N NMR (DMSO-d_6, 81 MHz), δ: −114.45, −53.58, −45.81, −44.00, 8.650; IR (KBr, cm^{-1}), υ: 3154, 3135 (−CH), 1530, 1390, 1331 (−NO$_2$), 1215, 1136, 1027 (pyrazole ring); Anal. calcd. for $C_6H_2N_{10}O_8$: C 21.06%, H 0.59%, N 40.94%; found C 21.08%, H 0.57%, N 40.92%. MS (APCI-) m/z: 377.18 [M+Cl]$^-$.

3   Results and Discussion

3.1 Synthesis

O-Mesitylenesulfonylhydroxylamine (MSH) is not stable in storage; it was therefore prepared from mesitylenesulfonyl chloride and ethyl acetohydroxamate as starting materials by condensation and hydrolysis before each amination reaction (Scheme 4). 1-Amino-3,5-dinitropyrazole (ADNP) was obtained by adding an acetonitrile solution of MSH to an acetonitrile solution of the potassium salt of 3,5-dinitropyrazole (DNPK) (Scheme 5).

In order to obtain ABDNP (10), 1-amino-3,5-dinitropyrazole (ADNP) was treated with different oxidizing agents as azo coupling reagents, following the synthetic procedures used for the generation of compounds 5-9 (Scheme 3). A range of different oxidants, which had been successfully used to prepare compounds containing the C−N=N−C structure from energetic compounds with a C−NH$_2$ group, were selected. Unfortunately, the formation of compound 10 was only observed when the oxidants t-BuOCl, SDCI or TCICA (Table 1) were used. The oxidative coupling reaction of ADNP indicates that the oxidants used are very specific for the yield of the product.

Scheme 4. Synthesis of *O*-mesitylenesulfonylhydroxylamine (MSH)
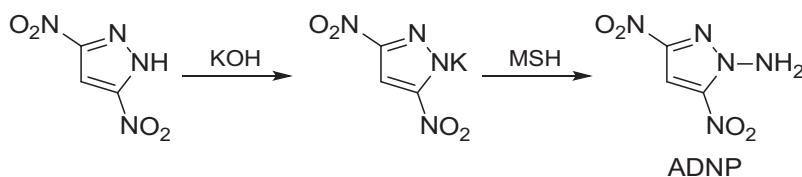
Scheme 5. Synthesis of 1-amino-3,5-dinitropyrazole (ADNP)

Table 1. Azo coupling reaction of 1-amino-3,5-dinitropyrazole with different oxidants

Entry	Reaction conditions					
	Oxidant	Solvent	Mol ratio[a]	Temperature [°C]	Time [h]	Yield [%]
1	t-BuOCl	CH_3CN	1:1.25	25	1	43.5
2	t-BuOCl	$CH_3COC_2H_5$	1:1.3	−5	3	11.8
3	SDIC	CH_3CN/H_2O	1:1.1	0	1	33.6
4	TCICA	CH_3CN/H_2O	1:1.1	0	1	38.1
5	$KMnO_4$/NaOH	H_2O	1:1	55	7	0
6	$KMnO_4$/HCl	H_2O	1:1	55	7	0
7	10% NaClO	H_2O	1:1	25	3	0
8	50% H_2O_2	CH_3CN/H_2O	1:1	25	7	0

[a] Mol ratio of 1-amino-3,5-dinitropyrazole and oxidant

3.2 X-Ray crystallography

A single crystal of compound ABDNP·2DMSO suitable for crystal structure analysis was obtained by slow evaporation from a DMSO solution of ABDNP at room temperature. The crystal data and structure refinement details of ABDNP·2DMSO are given in Table 2.

The crystal structure of ABDNP·2DMSO adopts a planar structure with two almost planar dinitropyrazole rings, a planar N₆ chain and an *E* configuration

about the azo bond plus two molecules of DMSO (Figure 1). The azo bond adopts a stable E configuration due to its lower active energy than the Z configuration. The bond length between the N-atoms of the azo group was 1.226 Å, shorter than that of compound 5 with the N_4 structure (1.249 Å), compound 6 with the N_8 structure (1.250 Å) and compound 9 with the N_{10} structure (1.243 Å), which indicates a stronger delocalization of the nitro π_3^4 conjugated bond and the azo π-bond along the molecular structure within compound 10. It was however longer than that of N_4H_4 (2-tetrazene) [27] with the N_4 structure (1.205 Å) and compound 7 with the N_{10} structure (1.178 Å), respectively. This is probably due to the electron-withdrawing property of the nitro group.

Table 2.   Crystal data and structure refinement details of ABDNP·2DMSO

|	
Empirical formula	$C_{10}H_{14}N_{10}O_{10}S_2$
Temperature	296(2) K
Wavelength	0.071073 nm
Crystal system	*Orthorhombic*
Space group	*Pca2(1)*
	$a = 1.12364(16)$ nm, $\alpha = 90°$
Unit cell dimensions	$b = 0.86163(13)$ nm, $\beta = 90°$
	$c = 2.1724(3)$ nm, $\gamma = 90°$
Volume	2.1032(5) nm^3
Z	4
Calculated density	1.574 g·cm^{-3}
Absorption coefficient	0.325 mm^{-1}
$F(000)$	1024
Crystal size	$0.38 \times 0.30 \times 0.25$ mm
Theta range for data collection	2.36° to 25.10°
Limiting indices	$-13 \leq h \leq 10$, $-10 \leq k \leq 9$, $-25 \leq l \leq 25$
Reflections collected/unique	9897/3700 [$R_{int} = 0.0291$]
Completeness to $\theta = 25.10$	99.9%
Max. and min. transmission	0.9223 and 0.8876
Goodness-of-fit on F^2	1.059
Final R indices *(I > 2σ(I))*	$R_1 = 0.0655$, w$R_2 = 0.1614$
R indices (all data)	$R_1 = 0.0761$, w$R_2 = 0.1702$
CCDC	1015098
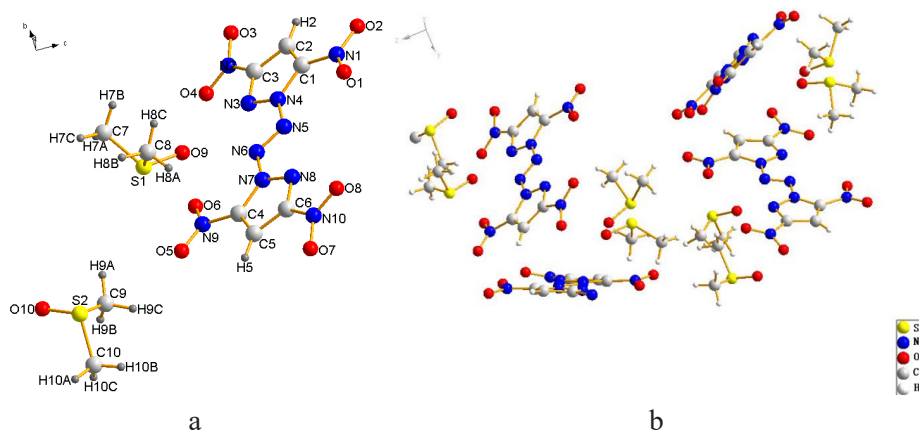
Figure 1. (a) Thermal ellipsoid plot of ABDNP·2DMSO (50% probability); (b) Packing diagram of ABDNP·2DMSO

3.3 Differential scanning calorimetry (DSC)

DSC measurements to determine the thermal behaviour of compound ABDNP were carried out with a heating rate of 5 °C·min⁻¹ using dry oxygen-free nitrogen as the atmosphere, at a flow rate of 20 mL·min⁻¹. A typical DSC thermograph of ABDNP is shown in Figure 2, with the temperature range 25-400 °C. Compound ABDNP was thermally stable to 202.9 °C, and an exothermic peak of thermal decomposition was observed at 239.6 °C. Its decomposition temperature is much higher than those of hexazene (N_6) ligand (140 °C) [28] and N_5^+ (70 °C) [29]. The thermal stability of compound ABDNP is also comparable with that of the traditional energetic compound RDX (244 °C) and superior to the other derivatives with more catenated nitrogen atoms (6, 193.8 °C; 7, 80 °C; 9, 127.2 °C). The delocalized π-system in the molecule probably accounts for the remarkable stability of this compound. Obviously, we can see from Table 3 that the larger the number of directly linked nitrogen atoms that are present in the system, the easier it is to be decomposed.
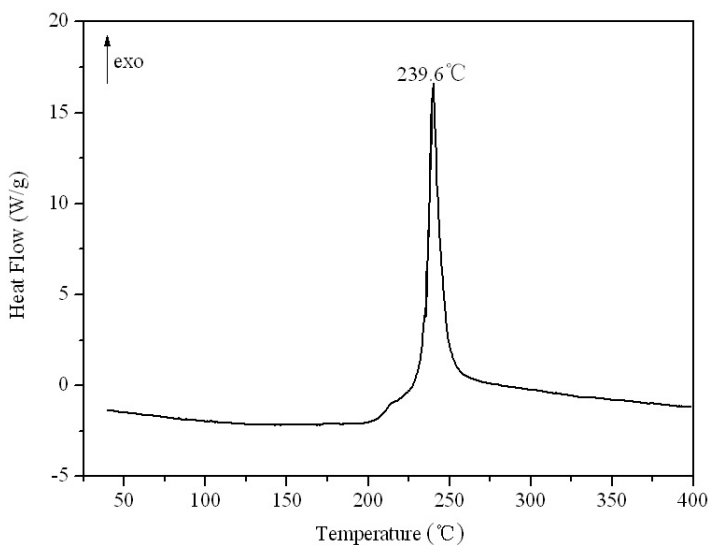
Figure 2.   DSC thermogram of ABDNP

3.4 Theoretical study

The geometries of all compounds were optimized at the B3LYP/6-31+G (d, p) level using the default convergence criteria and were confirmed to be true local energy minima on the potential energy surfaces, without imaginary frequencies. All calculations were carried out using the Gaussian 09 program [30].

The enthalpies of formation of the related compounds mentioned in this paper were computed by using an isodesmic reaction [31]. However, delocalized bonds which are separated in an aromatic molecule or cage structure, ordinarily cause errors in an isodesmic reaction. In order to obtain an accurate enthalpy of formation, the conjugated ring structure of the pyrazole was reserved and the isodesmic reaction of the azo compound was carried out according to Abou-Rachid (Scheme 4) [32]. The isodesmic reaction of ABDNP was designed as shown in Scheme 6. Based on the optimized structures, the total energy (E_0) and thermodynamic parameters, including zero point energy (ZPE) and thermal correction to the enthalpy (H_{corr}), were obtained at MP2(full)/6-311++G (d,p) level, and then the enthalpy of the isodesmic reaction could be obtained.
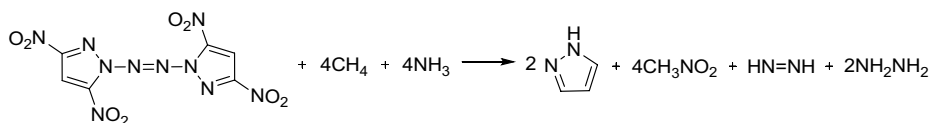
Scheme 6. Isodesmic reaction for compound ABDNP

3.5 Density, enthalpy of formation and detonation parameters

The performance of an energetic compound is mainly a function of the heat of formation of the compound and its density. The detonation pressure is dependent on the square of the density and the detonation velocity is proportional to the density [33]. Both of these parameters are governed by the compound's molecular structure. A higher density, heat of formation and nitrogen content are all directly related to the performance of a compound [34].

Density is one of the most important physical properties of an energetic compound. The structure of ABDNP was optimized by the Gaussian 09 program in order to obtain its stable geometric configuration. Its density was then calculated as 1.823 g·cm^{-3}, which compares with the measured value (1.824 g·cm^{-3}) by gas pycnometry. The density falls in the range for high-performance energetic materials (1.8-2.0 g·cm^{-3}) [35] and is superior to that of TNT (1.65 g·cm^3). The heat of formation is another important parameter that needs to be considered when designing new energetic compounds. The heat of formation of ABDNP was predicted based on its stable geometric configuration. As shown in Table 3, the results show that ABDNP (267.9 kJ·mol^{-1}) exhibits a higher positive heat of formation than that of RDX (92.6 kJ·mol^{-1}) and HMX (104.8 kJ·mol^{-1}).

Oxygen balance (OB), an expression used to indicate the degree to which an explosive can be oxidized, is an important index for identifying the potential of energetic materials as explosives or oxidants. Compound 10 has a negative oxygen balance of −23.4%, which is higher than other reported catenated nitrogen energetic compounds with N,N'-azo linkages, except for compound 8 (0%), better than traditional energetic materials such as TNT (−74.0%), and comparable with RDX (−21.6%) and HMX (−21.6%).

The properties of energetic compounds are measured by their detonation velocity and detonation pressure. These parameters are directly related to the density and the enthalpy of formation. The detonation parameters of ABDNP were calculated using the Gaussian 09 program and the empirical Kamlet-Jacobs equations [33a]. The calculated detonation pressure and detonation velocity of ABDNP were 30.5 GPa and 8.18 km·s^{-1} respectively, which are superior to those of TNT (19.5 GPa, 6.88 km·s^{-1}). The performance parameters of ABDNP and other reported nitrogen-rich energetic compounds, and compared with TNT, RDX and HMX, are listed in Table 3.

Table 3.   Properties of nitrogen-rich energetic compounds with an N,N'-azo linkage

Property	10	5	6	7	8	9	TNT [36]	RDX [37]	HMX [37]
F [a]	$C_6H_2N_{10}O_8$	$C_4H_4N_8$	$C_4H_4N_8$	$C_2H_2N_{10}$	$C_2N_{12}O_4$	$C_4H_6N_{10}$	$C_7H_5N_3O_6$	$C_3H_6N_6O_6$	$C_4H_8N_8O_8$
T_m [b]	-	-	-	-	50	-	80.4	203	276
T_d [c]	202.9	275.0	187.5	80 [m]	50	112.5	295	204.0	280.9
D [d]	1.82	1.60	1.62	1.77	1.80	1.48	1.65	1.82	1.91
OB [e]	−23.4	−97.6	−97.6	−48.2	0	−90.7	−74.0	−21.6	−21.6
N [f]	40.9	68.3	68.3	84.3	65.6	72.1	18.5	37.8	37.8
HOF [g]	267.9	861.4	962.3	1030.0	1153.0	986.1	95.3	92.6	104.8
P [h]	30.5	22.7	25.2	36.1	39.0	21.0	16.5	33.7	39.6
V_d [i]	8.18	7.43	7.76	9.18	9.18	7.32	6.88	8.71	9.01
IS [j]	6.0	14.0	4.1	<<1	<<<<1	-	39.2 [n]	5.9 [n]	6.4 [n]
FS [k]	60	-	-	<<5	<<<<5	-	360	120	112
ESD [l]	0.15	-	-	0.015	-	0.005	-	0.2	0.2

[a] Molecular formula; [b] Melting point (°C); [c] Thermal decomposition temperature (onset temperature at a heating rate of 5 °C·min^{-1}); [d] Density (g·cm^{-3}); [e] CO_2 oxygen balance (OB) is an index of deficiency or excess of oxygen in a compound required to convert all C into CO_2 and all H into H_2O. For compounds with the molecular formula of $C_aH_bN_cO_d$, OB (%) = 1600[(d-a-b/2)/M_w], M_w molecular weight of compound; [f] Nitrogen content (%); [g] Heat of formation (kJ·mol^{-1}); [h] Detonation pressure (GPa); [i] Detonation velocity (km·s^{-1}); [j] Impact sensitivity (J) (BAM drop-hammer, 1 of 6); [k] Friction sensitivity (N) (BAM friction tester, 1 of 6); [l] Electrostatic discharge sensitivity (J); [m] Thermal decomposition peak temperature (at heating rate of 5 °C·min^{-1}); [n] Reference [38].

4   Conclusions

(1) A catenated N$_6$, polynitro energetic compound: 1,1'-azobis(3,5-dinitropyrazole) (ABDNP) was synthesized, and its structure was characterized by IR spectroscopy, ^{1}H and ^{13}C NMR spectroscopy, elemental analysis and mass spectrometry.

(2) The thermal behaviour of ABDNP was studied using DSC. The thermal decomposition onset temperature of ABDNP was found to be 202.9 °C, which is comparable with that of the traditional energetic compound RDX and superior to most of the other derivatives with more catenated nitrogen atoms. The results show that this compound has acceptable thermal stability.

(3) The heat of formation and detonation properties of ABDNP were calculated using the Gaussian 09 program and the empirical Kamlet-Jacobs equations. ABDNP exhibited a higher positive heat of formation than RDX and HMX. The detonation velocity and detonation pressure are superior to those of TNT.

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