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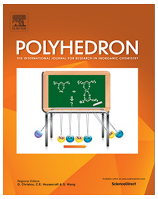

Insight into the thermostability and low sensitivity of energetic salts based on planar fused-triazole cation

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ABSTRACT

A new family of nitrogen-rich fused-triazole energetic salts based on 3,6-diamino-1H-[1,2,4]triazolo[4,3-b][1,2,4]triazole were synthesized and fully characterized by infrared spectroscopy (IR), ^1H and ^{13}C nuclear magnetic resonance, elemental analysis, differential scanning calorimetry (DSC). Structures of **3** and **4**·H_2O were confirmed by single-crystal X-ray diffraction analyses and their crystal packing characteristics were thoroughly analysed. All new compounds show good thermal stability (T_d > 223 °C) and tend to be insensitive to external mechanical stimulus. The densities of these salts ranged from 1.72 to 1.93 g cm^{-3}. Theoretical performance calculations (Gaussian 09 and EXPLO 5) provided detonation pressures and velocities within the ranges of 20.8 to 32.9 GPa and 7599 to 8719 m s^{-1}, respectively. The perchlorate salt **3** exhibits the highest density (1.93 g cm^{-3}) and best oxygen balance (−30.0%), good thermal stability (T_d = 258 °C), low sensitivities, and excellent detonation velocity (8719 m s^{-1}) and pressure (32.9 GPa), which suggest that it has the potential to be used as High-energy–density material.

1. Introduction

From the traditional explosive TNT (2,4,6-trinitrotoluene) to energetic salts of pentazolate anion (*cyclo*-N_5^-) [1], the development of energetic materials has been a continuously growing research topic for their academic and practical interests [2]. The design and synthesis of new nitrogen-rich heterocyclic compounds have been at the forefront of high-energy research, as they usually possess green decomposition products and high positive heats of formation (HOF) resulting from the large number of N—C/N single and double bonds [3]. Moreover, intra-/intermolecular hydrogen bonds formed in nitrogen-rich compounds would improve the density and decrease the sensitivity [4].Scheme 1.Scheme 2.

Compared to the non-fused ring analogues, nitrogen-rich fused heterocyclic compounds recently have attracted great attention due to the stronger delocalization effect of electron cloud, more rigid molecular structure and larger ring strain energy, which should lead to a higher density and superior performance [5]. Five/six-membered heterocycles have widely been employed in many fused compounds due to their high positive HOF and excellent stability, among which, 1,2,4-triazole is frequently used as a favorite building block for construction of high-energy–density materials (HEDMs) [6], such as 2,5-dinitramide-7-amino-[1,2,4]triazolo[1,5-a][1,3,5]triazine [7] and 4-amino-3,7-dinitrotriazolo[5,1-c][1,2,4]triazine 4-oxide [8]. Developing from monocyclic triazole to [1,2,4]triazolo[4,3-b][1,2,4]triazole, amino-substituted 1,2,4-triazoles proved to be excellent precursors for cations in energetic salts attributing to their high thermostability and low sensitivity, such as 4,4′,5,5′-tetraamino-3,3′-bi-1,2,4-triazolium dinitrate (T_d = 275 °C, impact sensitivity (IS) = 15 J) [9] and 3,6,7-triamino-7*H*-[1,2,4]triazolo[5,1-*c*][1,2,4]triazol-2-ium nitrate (T_d = 279 °C, IS = 40 J) [10].

Although 3,6-diamino-1*H*-[1,2,4]triazolo[4,3-*b*][1,2,4]triazole (**2**, DATT) has been reported just now [11], the intense interactions in its salts have barely been studied which are supposed to be the pivotal feature leading to good thermal stability and low sensitivity. Our research group had independently obtained DATT and its salts with higher yields almost at the same time, herein we reported five other energetic salts based on the planar fused-triazole cation of DATT. All of the compounds were fully characterized

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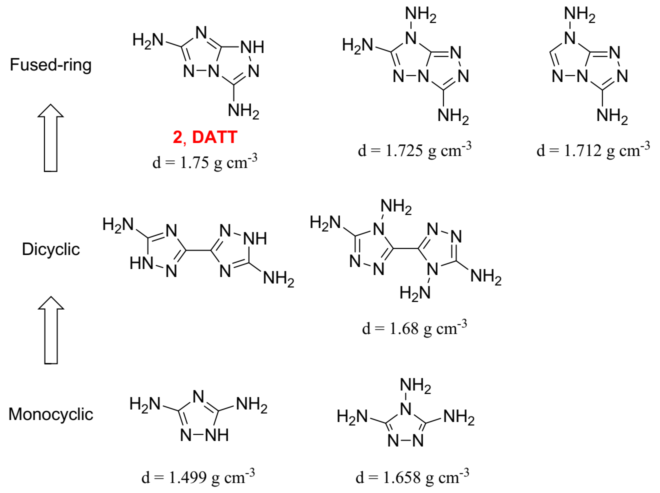


Scheme 1. Polyamine-triazole nitrogen-rich heterocyclic compounds.

and their detonation properties were calculated. Structures of **3** and **4**·H_2O were confirmed by single-crystal X-ray diffraction analyses and the intense interactions in them were thoroughly analysed.

2. Experimental section

Caution! Although we have not encountered any difficulties in handling these energetic materials, small scale and best safety practices (leather gloves and face shield) are strongly encouraged!

2.1. General methods

^1H, ^{13}C NMR spectra were recorded at 25 °C on a 600 MHz nuclear magnetic resonance spectrometer operating at 600 and 150 MHz, respectively. Chemical shifts are reported relative to TMS for ^1H and ^{13}C NMR spectra. The solvent was [D$_6$] dimethyl sulfoxide ([D$_6$]DMSO) unless otherwise specified. The melting and decomposition points were recorded on a differential scanning calorimetry (DSC) and a Netzsch Sta449F3 equipment at a heating rate of 5 °C min^{-1} in a dynamic nitrogen atmosphere (flow rate = 50 mL min^{-1}). The infrared spectra were recorded using KBr pellets. Densities were measured at 25 °C using a Micromeritics Accupyc Ⅱ1340 gas pycnometer. Elemental analyses were obtained on an Elementar Vario Micro Cube (Germany) elemental analyzer. The sensitivities to impact (IS) and friction (FS) were determined according to BAM standards [11].

2.2. Synthesis

2.2.1. 3,6-Diamino-1H-[1,2,4]triazolo[4,3-b][1,2,4]triazole (2, DATT)

3-Amino-5-hydrazino-l,2,4-triazole dihydrochloride (**1**) was prepared according to the literature[12]. A solution of **1** (1.87 g, 10 mmol) and cyanogen bromide (1.27 g, 12 mmol) in aqueous methanol (42 mL, 85%) was refluxed for two days. Methanol was removed by evaporation, the solid residue was filtered and then dispersed in proper water. The suspension system was neutralized by sodium hydroxide and then recrystallized to give light brown crystals (1.17 g, 84%). ^1H NMR: δ = 11.55 (s, 1H), 6.11 (s, 2H), 5.55 (s, 2H) ppm. ^{13}C NMR: δ = 170.25, 155.72, 141.73 ppm. MS (ESI): 140.15 (M + H)$^+$, 281.15 (M + H + MeCN)$^+$. IR (KBr pellet): 3694, 3414, 3331, 3149, 2785, 1686, 1647, 1617, 1587, 1541, 1490, 1439, 1398, 1356, 1254, 1183, 1133, 1087, 1011, 882, 846, 750, 714, 680, 625, 601, 415 cm^{-1}.Anal. Calcd. (%) For $C_3H_5N_7$: C, 25.90; H, 3.62; N, 70.48; found: C, 25.95; H, 3.61; N, 70.43.

2.2.2. General procedure for synthesis of 3–7

DATT (2 mmol) was dispersed in 40 mL water at room temperature followed by adding one equivalents of free acid (nitric acid (68%) or perchloric acid(70%)) in one portion. After stirring at 50 °C for 4 h, the solvent was evaporated in vacuo and the residue was crystallized from water (for **4**–**7**) or ethyl alcohol (for **3**).

2.2.3. 3,6-Diamino-7H-[1,2,4]triazolo[4,3-b][1,2,4]triazol-2-ium perchlorate (3)

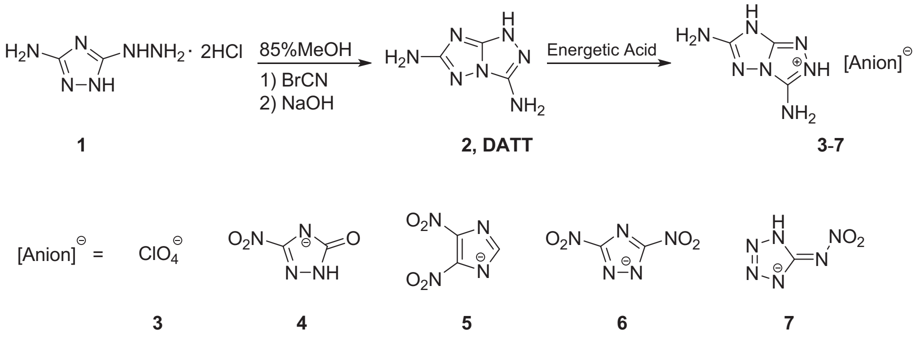
Colourless crystals (359 mg, 75% yield). ^1H NMR: δ = 13.18 (d, br, 2H), 8.08 (s, 2H), 7.07 (s, 2H) ppm. ^{13}C NMR: δ = 160.15, 148.76, 140.99 ppm. IR (KBr pellet): 1675, 1586, 1566, 1515, 1447, 1404, 1330, 1265, 1145, 1089, 941, 831, 718, 627, 492, 426 cm^{-1}.Anal. Calcd. (%) For $C_3H_6ClN_7O_4$: C, 15.04; H, 2.52; N, 40.92; found: C, 14.99; H, 2.61; N, 40.89.

2.2.4. 3,6-Diamino-7H-[1,2,4]triazolo[4,3-b][1,2,4]triazol-2-ium 3-nitro-5-oxo-1,2,4-triazolate (4)

Pale brownish-yellow crystals (479 mg, 89% yield). ^1H NMR: δ = 12.83 (s, 1H), 6.20 (s, 2H), 5.63 (s, 2H) ppm. ^{13}C NMR: δ = 169.10, 156.06, 154.91, 149.78, 141.63 ppm. IR (KBr pellet): 3561, 3476, 3404, 3209, 1673, 1614, 1548, 1509, 1390, 1356, 1311, 1174, 1052, 1020, 974, 835, 780, 729, 629, 603, 542, 419 cm^{-1}.Anal. Calcd. (%) For $C_5H_7N_{11}O_3$: C, 22.31; H, 2.62; N, 57.24; found: C, 22.37; H, 2.59; N, 57.17.

2.2.5. 3,6-Diamino-7H-[1,2,4]triazolo[4,3-b][1,2,4]triazol-2-ium 4,5-dinitroimidazolate (5)

Yellow solid (552 mg, 93% yield). ^1H NMR: δ = 7.76 (s, 2H), 7.21 (s, 2H) ppm. ^{13}C NMR: δ = 161.65, 149.83, 141.11, 139.75, 139.07, 138.82 ppm. IR (KBr pellet): 3607, 3526, 3400, 3174, 1682, 1657, 1620, 1592, 1536, 1510, 1449, 1352, 1303, 1244, 1179, 1098,



Scheme 2. Synthetic route of compounds **2**–**7**.

1012, 979, 895, 875, 860, 815, 753, 706, 682, 622, 603, 508, 424 cm^{-1}.Anal. Calcd. (%) For $C_6H_7N_{11}O_4$: C, 24.25; H, 2.37; N, 51.84; found: C, 24.27; H, 2.33; N, 51.89.

2.2.6. 3,6-Diamino-7H-[1,2,4]triazolo[4,3-b][1,2,4]triazol-2-ium 3,5-dinitro-1,2,4-triazolate (6)

Yellow solid (513 mg, 86% yield). ^1H NMR: δ = 13.20 (s, br, 2H), 8.05 (s, 2H), 7.06 (s, 2H) ppm. ^{13}C NMR: δ = 163.29, 160.04, 148.67, 140.98 ppm. IR (KBr pellet): 3304, 3164, 1680, 1553, 1500, 1450, 1394, 1360, 1306, 1116, 1056, 986, 846, 652, 559, 416 cm^{-1}.Anal. Calcd. (%) For $C_5H_6N_{12}O_4$: C, 20.14; H, 2.03; N, 56.37; found: C, 20.18; H, 2.13; N, 56.32.

2.2.7. 3,6-Diamino-7H-[1,2,4]triazolo[4,3-b][1,2,4]triazol-2-ium 5-nitriminotetrazolate (7)

White solid (452 mg, 84% yield). ^1H NMR: δ = 12.86 (s, 2H), 7.85 and 7.07 (d, br, 4H) ppm. ^{13}C NMR: δ = 160.70, 157.76, 149.11, 141.05 ppm. IR (KBr pellet): 3402, 3348, 3266, 3143, 2671, 1684, 1649, 1598, 1544, 1512, 1486, 1445, 1320, 1263, 1241, 1155, 1110, 1081, 1037, 1010, 889, 827, 767, 745, 689, 610, 551, 484, 444, 415 cm^{-1}.Anal. Calcd. (%) For $C_4H_7N_{13}O_2$: C, 17.85; H, 2.62; N, 67.64; found: C, 17.92; H, 2.59; N, 67.60.

3. Results and discussion

In contrast to the literature [11], 85% aqueous methanol was employed as solvent instead of dilute hydrochloric acid, in which 3-amino-5-hydrazino-l,2,4-triazole dihydrochloride (**1**) reacted with cyanogen bromide to obtain DATT with a higher yield of 84%. Subsequently, a series of energetic salts (**3**–**7**) were prepared from the reaction of DATT with the corresponding acid in water. All new compounds were dried at 60 °C under vacuum for 2 h before characterization by IR spectroscopy, differential scanning calorimetry (DSC), ^1H and ^{13}C NMR spectroscopy and elemental analysis. The data are listed in the Experimental Section.

The chemical shifts in the ^{13}C NMR spectra of DATT are identified at 170.25, 155.72 and 141.73 ppm, and the shifts for its cation are at around 160.45, 148.89, 141.05 ppm. The signal at δ = 11.55 ppm in ^1H NMR spectra of DATT is assigned to the NH in the fused-triazole backbone, while the rest peaks at 6.11 and 5.55 ppm are attributed to two amino groups. It's worth noting that all the signals of the caitons are slightly shifted downfield relative to those of DATT. The NMR chemical shifts of the anions **4**–**7** are consistent with those of the previously published ones [6f,10].

3.1. Crystal structure analysis

The X-ray quality crystal of **3** was obtained by slowly evaporating the ethanol at room temperature while **4**·H_2O was obtained from water. All the crystallographic data in this paper are attached in the supporting information as well as the reported crystal structures of DATT (**2**) and its 3,4,5-trinitropyrazolate salt which have also been obtained in our study. It's worth noting that both salt **3** and **4**·H_2O show face-to-face stacking structure which are supposed to obtain higher density compared to the crossing stacking structure of DATT and wave-like stacking structure of 3,4,5-trinitropyrazolate salt.

Salt **3** crystallized in the triclinic space group *P*1 with a calculated density of 1.939 g cm^{-3} at 150(2) K. The salt was formed by transfer of one proton from perchloric acid to precursor **2** and synchronous tautomerism of N1 = *C*2–N5 moiety, thus two hydrogen atoms are present at N1 and N4 positions in the cation which show broad double peaks at around 13.18 ppm in ^1H NMR spectra. All atoms in the cation are coplanar with the largest torsion angle of −176.4(2)° between N2–N3–C3–N4 while the dihedral angles between triazole and two amino groups (2.78° and 0.60°, respectively) are much smaller than those of **2**. The bond lengths of C1–N6 and C3–N7 are 1.340(3) and 1.320(3) Å, respectively, which are slightly shorter than those of **2**, thus indicate strong conjugation effect throughout the cation. The lengths of hydrogen bonds among cations vary from 2.981 Å (N7–H7A···N4) to 3.465 Å (N6–H6B···N3) and are much shorter than those in **4**·H_2O. As shown in Fig. 1b, strong hydrogen bonds linked to O1 of perchlorate with N—H of cations in the upper layer looks like funnels, and their lengths lie in the range between 2.363 (N1–H1···O1) and 3.069 Å (N7–H7B···O1). It is critical that O2–O3–O4 in perchlorate anions almost lie in the same plane of its paired cations with a small deviation of 4.02°, thus anions seems to be embedded in the face-to-face stacking of cations. The strongest hydrogen bonds are observed between perchlorate and its surrounding cations in the same layer with the lengths varying from 2.009 Å to 2.607 Å (Fig. 1c). Attributing to the abundant hydrogen bonds, the discrete anions and cations are firmly linked into a 3D network. The layer distance in the compact packing structure consequently decreased to 3.123 Å and led to the highest density among the energetic salts of DATT.

Compound **4**·H_2O crystallized in the monoclinic space group P2$_1$/c with a calculated density of 1.772 g cm^{-3} at 167(2) K. The unit contains one fused-triazole cation, one 3-nitro-5-oxo-1,2,4-triazolate anion and one H_2O molecule. The bond lengths of C1–N6 and C3–N7 are 1.320(3) and 1.329(3) Å, respectively. The dihedral angles between triazole and two amino groups are 1.30° and 1.79°, respectively. The cations and anions are approximately parallel with a dihedral angle of 6.87°. As shown in Fig. 2b, the face-to-face stacking structure of **4**·H_2O was built up with a layer distance of 3.200 Å.

3.2. Stability

3.2.1. Thermal stability

Thermal stability is an important property to evaluate the application potential of energetic materials. As shown in Table 1, only perchlorate (**3**) and 4,5-dinitroimidazolate (**5**) salts melt prior to decomposition, having T_m = 244 and 130 °C, respectively. Decomposition temperatures of all new salts which range from 223 °C (**5**) to 258 °C (**3**) are lower than that of DATT (277 °C). Thus, energetic salts of DATT exhibit good thermal stabilities which are superior to that of 1,3,5-trinitro-1,3,5-triazinane (RDX, T_d = 204 °C).

3.2.2. Mechanical sensitivity

DATT (**2**) and its 3-nitro-5-oxo-1,2,4-triazolate salt (**4**) are classed as impact and friction insensitive energetic materials (IS > 40 J, FS > 360 N). Salts **3** and **5**–**7** are insensitive toward impact (IS > 40 J) and their FS values are higher than 216 N. All new compounds are much less sensitive than RDX (IS = 7 J, FS = 120 N).

3.3. Intermolecular interaction analysis

In order to further insight the causes of good thermal stability and low sensitivity of these energetic salts, non-covalent interaction (NCI) analysis [13], two-dimensional (2D) fingerprints and Hirshfeld surfaces analysis [14] of these compounds were performed.

The NCI plots of compound **3** and **4** are shown in Fig. 3. The face-to-face π-π interaction surfaces can be distinctly observed between parallel layers as green isosurfaces. Compared to salt **4** and 3,4,5-trinitropyrazolate salt, the larger isosurfaces in **3** indicate the more extensive π-π interaction in its packing structure, thus greatly improve the stability although perchlorate is usually a sensitive anion.

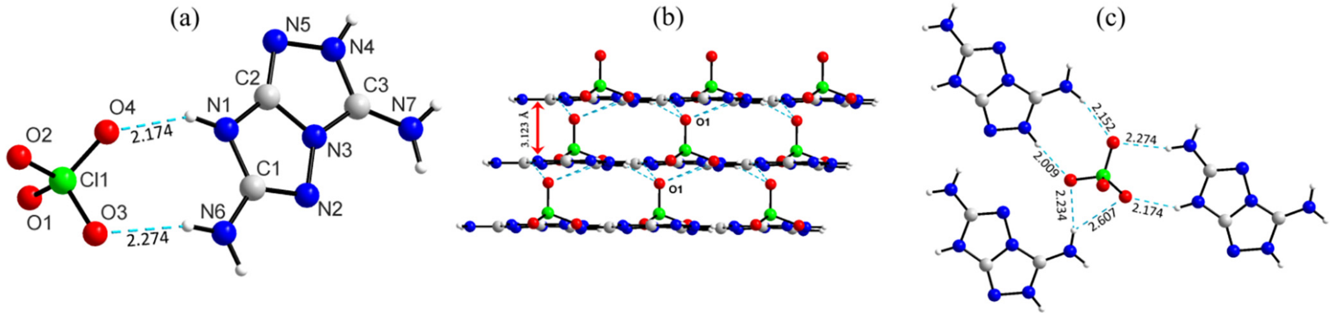


Fig. 1. (a) Crystal structure of compound **3**. (b) Packing diagram of **3** viewed towards plane h, k, l = −275, 51, 370. Only strong hydrogen bonds between O1 of perchlorate and N—H of cations are represented as blue dotted line for clarity. (c) Hydrogen bonds between perchlorate and its surrounding cations in the same layer.

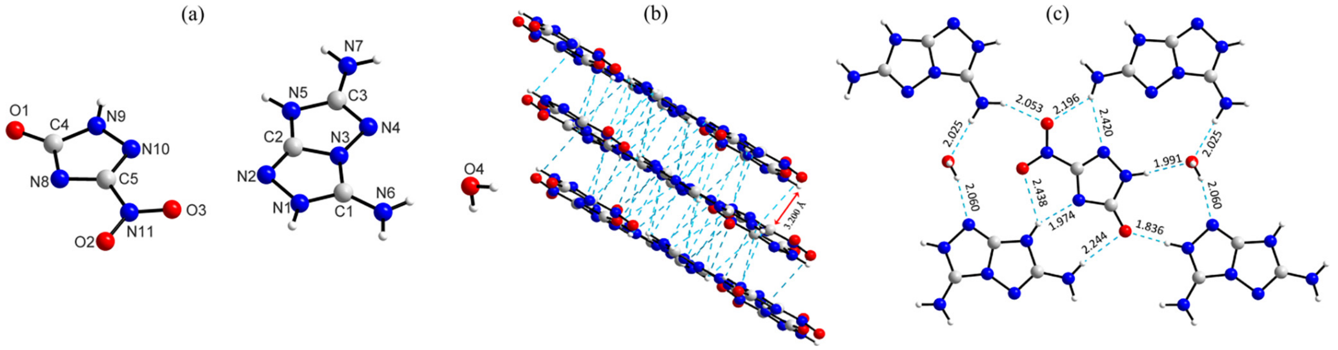


Fig. 2. (a) Crystal structure of compound **4**·H_2O. (b) Packing diagram of **4**·H_2O viewed towards plane h, k, l = 0, 1, 0. Blue dotted line represents hydrogen bonds between adjacent layers·H_2O molecules are omitted for clarity. (c) Hydrogen bonds between 3-nitro-5-oxo-1,2,4-triazolate and its surrounding cations/H_2O molecules in the same layer.

Table 1
Physical properties and thermochemical values of compounds **2**–**7**.

Comp.	2	3	4	5	6	7	RDX[k]
$T_m^{[a]}$ (°C)	dec	244	dec	130	dec	dec	dec
$T_d^{[b]}$ (°C)	277	258	240	223	232	244	204
$\rho^{[c]}$ (g cm^{-3})	1.75	1.93	1.77	1.73	1.72	1.73	1.80
N[d] (%)	70.5	40.9	57.2	51.8	56.4	67.6	37.84
OB[e] (%)	−97.7	−30.0	−62.4	−61.9	−48.3	−56.5	−21.6
$\triangle_f H_{sal}^{[f]}$ (kJ mol^{-1})	220.7	122.7	490.9	338.8	401.5	440	70.3
$v_D^{[g]}$ (m s^{-1})	7923	8719	7912	7599	7726	7831	8795
$P^{[h]}$ (GPa)	20.8	32.9	22.5	21.3	22.1	21.1	34.9
IS[i] (J)	>40	>40	>40	>40	>40	>40	7
FS[j] (N)	>360	216	>360	288	288	216	120

[a] Melting point. [b] Thermal decomposition temperature. [c] Measured density (gas pynometer). [d] Nitrogen content. [e] Oxygen balance. [f] Calculated molar enthalpy of formation of salts. [g] Detonation pressure. [h] Detonation velocity. [i] Impact sensitivity. [j] Friction sensitivity (BAM friction apparatus). [k] From Ref. [6b].

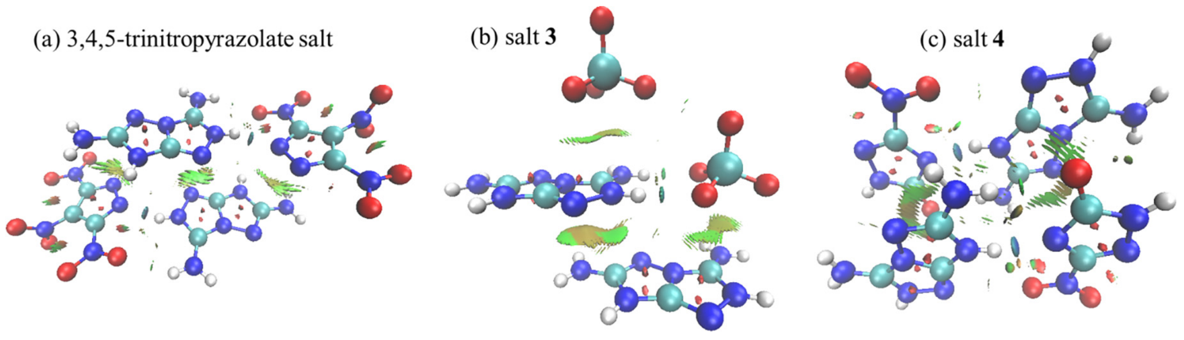

(a) 3,4,5-trinitropyrazolate salt (b) salt **3** (c) salt **4**

Fig. 3. π-π Interactions in 3,4,5-trinitropyrazolate salt, **3** and **4** (blue, strong attraction; green, weak interaction; red, strong repulsion).

To better understand their structure-performance, 2D fingerprint plot and Hirshfeld surface were employed to demonstrate the intermolecular interactions (Fig. 4). The red dots on the Hirshfeld surface are attributed to close contacts such O···H/H···O and N···H/H···N interactions. As shown in 2D fingerprint plots, these hydrogen bonds account for more than 60% of the total weak interactions, implying that hydrogen bonds are the primary driven force to construct these three self-assembled crystals. The blue regions on the Hirshfeld surface belong to π-π interaction, such as C — N, C — O and N — O interaction. Consistent with NCI analysis, compound **3** possesses the largest proportion of π-π interaction (19.8%) among three crystals, which would give rise to high density and low sensitivity especially when cooperated with hydrogen bonds.

3.4. Energetic performance

Density is the critical parameter contributing to the performance. DATT has a density of 1.75 g cm^{-3}, while the densities of its salts range from 1.72 (**6**) to 1.93 (**3**) g cm^{-3}. It is noteworthy that the density of perchlorate salt (**3**) is much higher than that of RDX (1.80 g cm^{-3}), and falls in the range of HEDMs (1.8–2.0 g cm^{-3}). In addition, salt **3** also possesses the best oxygen balance (OB = –30.0%).

Heat of formations were calculated by G4(MP2)-6X method [15] using the Gaussian 09 (Revision A.02) [16]. DATT has a positive HOF of 306.1 kJ mol^{-1}, whereas its cation possess a much higher value of 907.0 kJ mol^{-1}. HOFs of all salts are higher than that of RDX (70.3 kJ mol^{-1}) and rang from 122.7 (**3**) to 490.9 kJ mol^{-1} (**4**) as computed using the Born–Haber energy cycle.

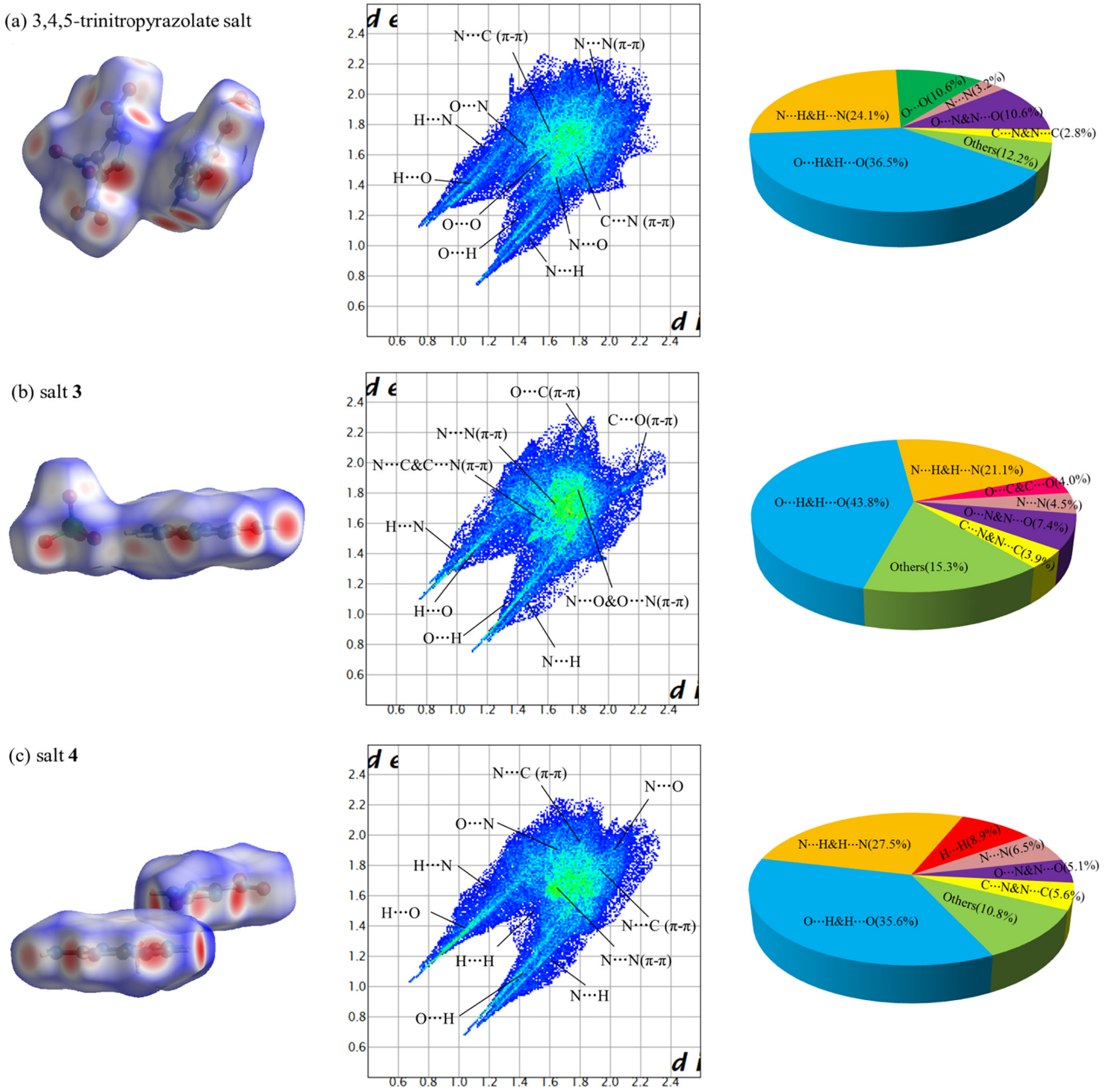


Fig. 4. Hirshfeld surfaces, 2D fingerprint plots and the individual atomic contact percentage contribution of 3,4,5-trinitropyrazolate salt, **3** and **4**.

Based on the density and HOF, the detonation pressures (*P*) and velocities (v_D) of all compounds were determined using the EXPLO5 program (Version 6.01) [17]. The detonation velocities range from 7599 to 8719 m s^{-1} and detonation pressure range from 20.8 to 32.9 GPa, which are superior to traditional military explosive TNT (v_D = 6881 m s^{-1}, *P* = 19.5 GPa). The perchlorate salt **3** exhibits the best detonation performance (v_D = 8719 m s^{-1}, P = 32.9 GPa) which is comparable to RDX (v_D = 8795 m s^{-1}, P = 34.9 GPa).

4. Conclusions

In this work, five energetic salts based on DATT were synthesized and fully characterized. The structures of salts **3** and **4**·H_2O have been analyzed by single-crystal X-ray diffraction analysis. All these compounds exhibit low sensitivity (IS > 40 J, FS $\geq$ 216 N) and good thermal stability with decomposition temperatures above 223 °C. The densities of all nitrogen-rich salts lie in the range between 1.72 and 1.93 g cm^{-3}. The calculated detonation velocities range from 7599 to 8719 m s^{-1} and detonation pressure range from 20.8 to 32.9 Gpa. According to 2D fingerprint, Hirshfeld surface and NCI analysis, extensive hydrogen bonds and impactful π-π interactions lead to low sensitivity (IS > 40 J, FS = 216 N) and the highest density (d = 1.93 g cm^{-3}) of perchlorate salt **3**, thus confirming its excellent detonation performance (v_D = 8719 m s^{-1}, P = 32.9 GPa) which is comparable to RDX. These advantages suggest that perchlorate salt **3** may well have promising applications as high-energy–density materials.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.poly.2021.115158.

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