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ARTICLE

Synthesis and characterization of three pyrazolate inner diazonium salts: green, powerful and stable primary explosives

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The synthesis and energetic performances of three inner diazonium salts, 3,5-dichloro-4-diazopyrazole zwitterion (**1**), 4-diazo-3,5-dinitropyrazole zwitterion (**2**), and 4-diazo-5-nitro-pyrazol-3-one zwitterion (**3**), were investigated in this study. All these compounds were characterized by IR, UV/Vis, ^{13}C, and ^{15}N NMR spectroscopy, and elemental analysis. Their structures were further confirmed by single crystal X-ray diffraction. Moreover, their themal stabilities are determined by differential scanning calorimetry (DSC). In addition, detonation parameters (e.g. detonation velocity and pressure) of the target compounds were computed using EXPLO 6.01 based on the calculated heat of formation and density. The results show that compound **2** exhibits a density of 1.849 g·cm^{-3} and a decomposition temperature (T_d) of 154 °C, which are superior to that of the efficient primary explosive DDNP (2-diazo-4,6-dinitrophenol, T_d= 142 °C). Compounds **1** and **3** also have moderately high decomposition temperatures of 135 and 151 °C, respectively. Besides, compounds **2** and **3** exhibit good detonation properties (**2,** 9038 m s^{-1}, 35.0 GPa; **3,** 8055 m s^{-1}, 26.4 GPa), which are higher than those of the widely used primary explosives DDNP (7290 m s^{-1}, 23.7 GPa) and $Pb(N_3)_2$ (5876 m s^{-1}, 33.4 GPa). The moderately high thermal stabilities combined with the good detonation properties make them potential green primary explosives.

Introduction

Primary explosives are an important class of energetic materials that are able to transition from deflagration to detonation and generate a shock wave, which makes the transfer of the detonation to a less sensitive secondary explosive.[1, 2] Until now, lead azide and lead styphnate are still the most widely used primary explosives.[3] For example, lead azide is widely used in detonators, electric igniters, and primary compositions to ignite burning.[4] However, the toxicity and the contamination caused by lead-based primary explosives are hazards that cause serious environmental and health issues.[5] Thus, considerable efforts have been made to develop green, lead-free substitutes that can be used as primary detonators, resulting in the synthesis of many candidates, such as copper(I) 5-nitrotetrazolate (DBX-1) [6] and potassium 1,1’-dinitramino-5,5’-bis-(tetrazolate) (K_2DNABT).[7] However, most of these substitutes contain metal elements, which could compromise their detonation properties. Therefore, there is an obvious demand for green, lead-free substitutes containing only CHON elements, which can be used as primary detonators.[8]

The chemistry of organic diazonium salts has been extensively studied over the past few decades for their practical value.[9-11] Diazonium salts are important intermediates and have found wide applications in organic synthesis. For example, many functional groups such as hydroxyl, halogen, and cyanide can be introduced by nucleophilic substitution on a diazonium salt, and diazonium salts can also be transformed to azo compounds.[12] More importantly, diazonium salts as lead-free substitutes, such as DDNP (Figure 1),[13, 14] which is used for charges in percussion caps and in detonators,[15] have exhibited extensive applications as primary explosives because they only contain CHON elements, which produce large amounts of gases during detonation, leading to materials with improved detonation properties. However, DDNP has the drawback of being less explosive than lead azide, which limits its application to some extent.[16] Consequently, it is necessary to make effort to find alternative substances with higher energy than DDNP.

In recent years, the study of heterocyclic energetic compounds has received considerable attention, as the energy of these compounds originates not only from the carbon oxidation of the

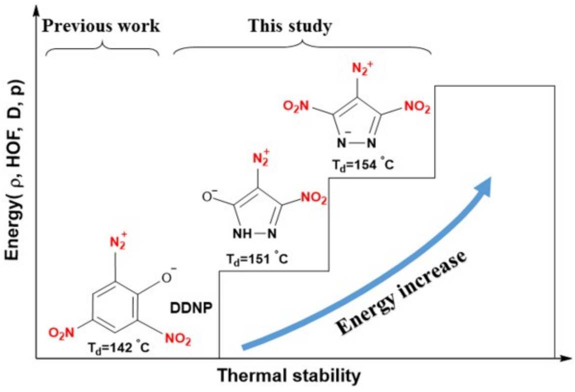

Figure 1. Structures of DDNP and substitutes for DDNP (DSC heating rate: 5 °C/min)

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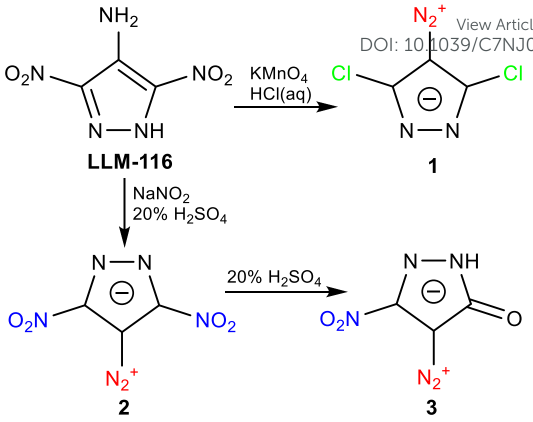
Electronic Supplementary Information (ESI) available: CCDC 938887-938889. For ESI and crystallographic data in CIF or other electronic format. See DOI: 10.1039/x0xx00000x ring but also from the inherent ring strain and high heats of formation,[17] which are rather different from those of aromatic energetic materials. Among them, pyrazolate inner diazonium salts can probably serve as substitutes of DDNP for the following reasons: (1) pyrazole is an attractive building block for energetic materials as already existing pyrazole-based compounds exhibit high densities and good thermal stabilities;[18] (2) they possess high nitrogen content, which results predominantly in the generation of environmentally benign nitrogen gas during detonation; moreover, the three carbon atoms in these molecules can be modified to further adjust their performances; (3) similarly to the aromatic DDNP, inner diazonium salts based on azotic heterocyclic compounds have good stabilities;[19-22] (4) azotic heterocyclic inner diazonium salts are easily prepared by neutralization of the corresponding diazonium compounds.[23]

Base on the above considerations, we envision that 4-diazo-3,5-dinitropyrazole zwitterion (Figure 1) could be employed as a lead-free, green alternative to the commonly used lead-based primary explosives and DDNP as it contains two energetic nitro groups that can further improve the density and therefore detonation properties of the compound. Additionally, it is easily obtained through simple diazotization of the well-known high energetic material LLM-116 (4-amino-3,5-dinitropyrazole). Despite being first prepared by Dalinger and coworkers in 1997,[24] to the best of our knowledge, the crystal characterization and energetic studies of 4-diazo-3,5-dinitropyrazole zwitterion have not been reported.

Herein we report the synthesis and characterization of inner diazonium salt 4-diazo-3,5-dinitropyrazole zwitterion (**2**). In order to study the effects of functional groups on the energetic properties, electron withdrawing substituents were bonded to the carbon atoms in the ring and thus two new compounds 3,5-dichloro-4-diazopyrazole zwitterion (**1**) and 4-diazo-5-nitro-pyrazol-3-one zwitterion (**3**) were synthesized and characterized. The structures of the three compounds were determined by single crystal X-ray diffraction, and their thermal stabilities and energetic properties were studies in detail.

Results and discussion

The synthetic routes to the target compounds are outlined in Scheme 1. The starting material, LLM-116, was prepared according to a literature procedure.[25] Generally, diazonium salts are synthesized by diazotization of the appropriate amine using $NaNO_2$ and strong acids. Compound **2** was synthesized by this conventional method and further oxidized into **3** using sulfuric acid. Surprisingly, diazonium salt **1** could be prepared by adding potassium permanganate and hydrochloric acid in the absence of $NaNO_2$. The structures for three target compounds were characterized by IR, UV/Vis, ^{13}C, and ^{15}N NMR spectroscopy, and single crystal X-ray diffraction.



Scheme 1. Synthesis of compounds **1**, **2** and **3**.

The IR spectrum for compound **1** shows a strong band at 2169 cm^{-1}, which is assigned to the diazo group ($N^+\equiv N$), while the IR spectrum of **2** shows a very strong peak at 2233 cm^{-1} attributable to the diazo group ($N^+\equiv N$). In addition, two peaks 1557 and 1347 cm^{-1} in the spectrum of **2** are assigned to the vibrations of the NO_2 groups. For compound **3**, the characteristic strong absorption band of the diazo group ($N^+\equiv N$) is observed at 2171 cm^{-1}, and the two intense absorptions at 1554 and 1357 cm^{-1} reveal the characteristic frequencies for asymmetric and symmetric vibrations due to NO_2 groups. Additionally, compound **3** exihibits a very strong peak at 1675 cm^{-1}, which is ascribed to the carbonyl group present in the molecule. The UV/Vis spectrum (Figure S5) shows that the maximum absorption wavelenghs for three compounds in acetonitrile are 244, 229, and 357 nm, respectively.

Compound **1** is symmetric and its ^{13}C spectrum shows signals at 80.5 and 143.5 ppm attributed to $C–N_2^+$ and C–Cl, respectively. Similarly, the resultant spectrum for compound **2** diaplays two sharp peaks at 76.6($C–N_2^+$) and 157.2($C–NO_2$) ppm. The carbon atoms for **3** appear at 104.5($C–N_2^+$), 164.1($C–NO_2$) and 174.7(carbonyl carbon) ppm. The cause of the chemical-shift variation in the ^{13}C NMR of **3** is the asymmetry of the molecular. The ^{13}C NMR spectra for three target compounds are given in the supplementary information.

The ^{15}N NMR for three target compounds were measured in Acetone-d_6 with respect to CH_3NO_2 as the external standard, and

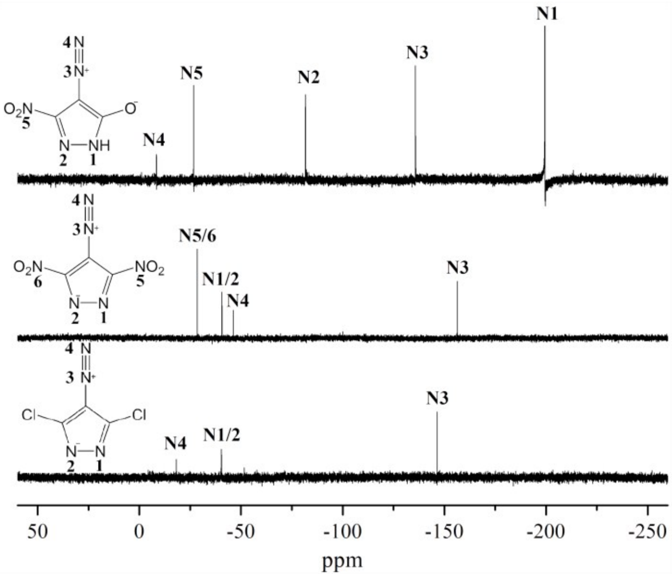


Figure 2. ^{15}N NMR spectra of **1**, **2** and **3**.

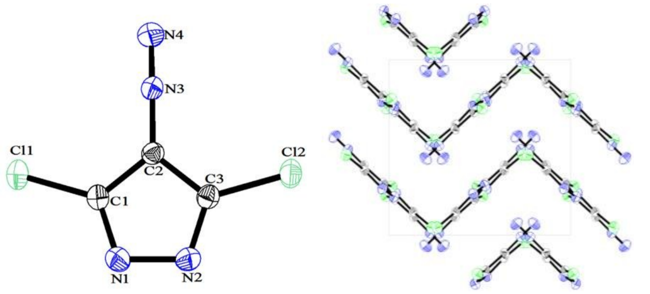


Figure 3. Left: Molecular structure of **1** (thermal displacement at 50% probability). Right: Packing diagram of **1**.

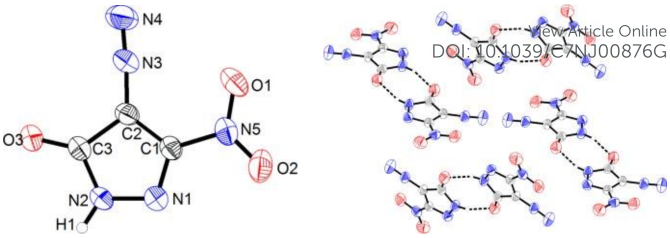


Figure 5. left: Molecular structure of **3** (thermal displacement at 50% probability). right: Packing diagram of **3**(the dashed lines indicate hydrogen bonding)

the spectra are given in Fig. 2. The assignments are based on the literature values of some pyrazole based compounds and diazonium salts.[26-29] The nitrogen atoms (**1**: δ = –40.35 ppm; **2**: δ = –40.62 ppm) in the pyrazole rings of **1** and **2** and the nitro groups (δ = –28.46 ppm) of **2** show a single peak, due to their symmetrical structure. However, two signals (N1: δ = –199.45 ppm; N2: δ = –81.69) of the ring for **3** were observed because of its unsymmetrical structure, and signal of nitro group appears at –26.67 ppm. The resonance sgnals of the positive charged diazonium nitrogens for **1**–**3** are found at high field (**1**: δ = –146.67ppm; **2**: δ = –156.35 ppm; **3**: δ = –135.79 ppm), while the terminal diazonium nitrogen atoms are detected at low field (**1**: δ = –18.17 ppm; **2**: δ = –46.24 ppm; **3**: δ = –8.41 ppm). The ^{15}N signals of nitrogen atoms in the pyrazole ring for **3** were found at δ = –81.69 (N2) and –199.45 (N1).

The crystal structures of compounds **1**–**3** were determined by X-ray diffraction. Tables S1–S2 in the supplementary information illustrate selected data and parameters of the X-ray measurements. These three compounds were crystallized from ethyl acetate by slow evaporation at room temperature. The CIF files were deposited with CCDC no. 1018388 (**1**), 1018387 (**2**), and 1018389 (**3**).

Compound **1** crystallizes in the orthorhombic space group Pbca with eight molecules per unit cell and with a density of 1.894 g·cm^{-3} at 153 K. Its high density may be attributable to the heavy Cl atom and intensive zigzag packing mode. The molecular structure and packing diagram of **1** is illustrated in Figure 3. The crystal data (see Table S1) shows that the C1–C2 (1.416 Å) and C2–C3 (1.414 Å) bond lengths in the pyrazole ring are in between that of the C–C single bond (1.54 Å) and the C=C double bond (1.34 Å). The C1–N1, C3–N2, and C2–N3 bond lengths are 1.304, 1.307, and 1.332 Å, respectively, which are closer to the standard bond length of the C=N double bond (1.28 Å) than to that of the C–N single bond (1.47 Å). The distance between N3 and N4 of the diazo moiety is 1.106 Å, which corresponds to a N≡N triple bond, and it is identical to those found in other inner diazonium salts.[19, 30] The dihedral angles are all close to either 0 or 180°, which indicates that all the atoms are almost coplanar. Figure 3 and the data in Table S1 suggest that the molecule is symmetric along C2–N3–N4, because the bilateral bond lengths and bond angles of C2–N3-–N4 are consistent.

Compound **2** crystallizes in the monoclinic space group P21/n with eight molecules per unit cell as well, and with two different molecular structures in the crystal, for which the crystal data are slightly distinct, leading to two types of perpendicular stacking modes. Its relatively high density at 153K (1.849 g·cm^{-3}) may be due to the two nitro groups in the molecule, because the density of the compound will increase significantly by introducing nitro groups. The diazo bond length, N3–N4 [1.098(14) Å], is also in the range of a N≡N triple bond. Noticeably, **1** and **2** are symmetric molecules and the only difference between them is the substituent groups at C1 and C3. Moreover, the data in Table S1 suggests that all atoms of **2** are also nearly coplanar.

Compound **3**, which was obtained from the oxidation of **2** with sulfuric acid, crystallized with the same crystal system and space group as **2**. The cell parameters of **3** are as follows: a = 5.536(4) Å, b = 9.134(7) Å, c = 11.526(8) Å; β = 91.852(6)°, α = γ = 90°. The C1–N1, C1–C2, N2–N1, C2–C3, and N2–C3 bond lengths are 1.294, 1.410, 1.366, 1.441, and 1.367 Å, respectively, which are common values in pyrazoles.[18, 31] The C3–O3 bond length is 1.227 Å and corresponds to that of a normal double bond length of a carbonyl group. The carbonyl group lies in the plane of the pyrazole ring (the torsion angle of N1–N2–C3–O3 is 179.2°), while the nitro group bonded to the pyrazole is twisted, with torsion angles of 7.83° for N1–C1–N5–O2 and 4.86° for C2–C1–N5–O1. The density of **3** decreases compared to that of **2**, as one -NO$_2$ group is substituted by a carbonyl group.

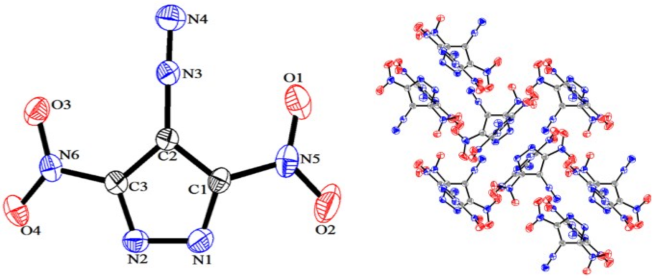


Figure 4. Left: Molecular structure of **2** (thermal displacement at 50% probability). Right: Packing diagram of **2**.

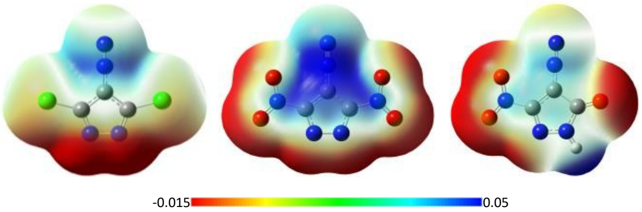


Figure 6. Electrostatic potential of compound **1**(left), **2**(middle) and **3**(right) [B3LYP/6-311++g(d,p), 0.001 electron/b^3 isosurface, energy values -0.0015 to +0.05 H]. Colour coding: dark red, very negative; yellow, slightly negative; green, neutral; turquoise, slightly positive; light blue, positive; dark blue, very positive.

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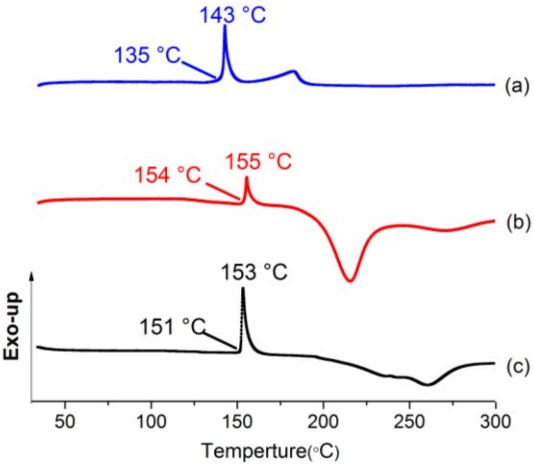

Figure 7. DSC comparison for three compounds, heating rate: 5 °C/min. (a) 3,5-dichloro-4-diazopyrazole zwitterion. (b) 4-diazo-3,5-dinitropyrazole zwitterion. (c) 4-diazo-5-nitro-pyrazol-3-one zwitterion.

The computed electrostatic potential (ESP) of the molecular surface (Figure 6) clearly reveals that there is obvious charge separation in these three molecules, that is, the positive charge is assembled in the diazo moiety, whereas the negative charge is delocalized around the pyrazolium rings, which confirms the zwitterionic nature of these structures.

In the molecular structure of **1**, Cl can be considered as oxidant while N_2^+ can be regarded as energetic group. As for **2**, besides the diazo group, the nitro substituent on the pyrazole backbone is also a common energetic group, while **3** contains the same functional groups as the widely used primary explosive DDNP. In summary, all three compounds can function as energetic materials, for this reason their energetic properties need to be fully investigated.

Among the various energetic parameters, thermal stability is the most important index of an energetic material, which directly determines its application.[32] Diazonium salts are known to be thermally unstable (for example, T_d for benzenediazonium chloride is 40 °C[33]; T_d for 2-nitrobenzenediazonium chloride is 60 °C[33]) and decompose losing the diazo functional group as nitrogen gas.[34] However, inner diazonium salts **1, 2,** and **3**, decompose, without melting, at relatively high temperatures (135, 154, and 151 °C, respectively, see Figure 7). Their relatively high thermal stabilities are a result of their zwitterionic structures, which greatly improve the conjugate effect between the pyrazole ring and diazo group, causing the diazo group to become more stable; moreover, the atoms of all three compounds are nearly coplanar, and these arrangements facilitate the formation of stable conjugated systems, eventually resulting in more stable molecules.

The heat of formation (HOF) is also an important parameter to evaluate the performance of energetic materials and can be calculated with good accuracy using isodesmic reactions of solid explosives.[35] The solid state HOFs for compounds **1**-**3** were calculated from their gas phase HOF and heat of sublimation presented in Tables S3 and S4 in the supplementary information. In general, the presence of either a nitro group or carbonyl group reduces the heat of formation of a compound.[36] However, compounds **1**-**3** possess positive HOFs, and **2** has the highest HOF value (407.8 kJ mol^{-1}) among them.

Besides the HOFs, Oxygen balance (OB) is another significant parameter of energetic materials. OB is used to indicate the degree to which an explosive can be oxidized. The OB values for compounds **1**, **2**, and 3 are all negative (-67.9, -17.4, and -36.1%, respectively). Noteworthy, molecule **1** contains chlorine atoms, which can be consider as oxidizers. However, as it contains no hydrogen atoms, the calculation method of OB for **1** is the same as that for **2** and **3**.

With the data of molecular weight, density, and heat of formation in hand, the detonation pressures (P) and velocities (v_D) of compounds **1**–**3** were calculated using EXPLO5 v6.01. As shown in Table 1, compound **1** (v_D = 5954 m s^{-1}) achieves slightly higher detonation velocity than $Pb(N_3)_2$ (v_D = 5876 m s^{-1}), but its detonation pressure is the lowest in the table. Although compound **2** has a similar symmetrical structure to **1**, it possesses a remarkable detonation performance (v_D = 9038 m s^{-1}, P = 35.0 GPa), due to the nitro groups, which improve the energetic properties and indirectly enhance the OB. Compound **3** has the same substituent groups as the widely used primary explosive DDNP, however, its detonation velocity (8055 m s^{-1}) and detonation pressure (26.4 GPa) are notable higher than those of DDNP (7290 m s^{-1}, 23.7 GPa). For safety considerations, their sensitivities toward impact and friction were determined using standard BAM technology. As all of these compounds contain diazo groups, it's no wonder that they diaplay high mechanical sensitivities. The impact sensitivities for **1**-**3** are comparable to that for $Pb(N_3)_2$, and they are also sensitive to friction. The data presented in Table 1 suggests that compounds **1**

Table 1. Physical properties of **1**-**3** compared with DDNP and $Pb(N_3)_2$

Compd.	T_d[a] [°C]	ρ[b] [g cm^{-3}]	OB[c] [%]	ΔH_f[d] [kJ mol^{-1}/kJ g^{-1}]	v_D [e] [m s^{-1}]	P[f] [GPa]	IS[g] [J]	FS[h] [N]
1	135	1.85	–58.9	355.2 / 2.18	5954	14.0	2.5	<5
2	154	1.81	–17.4	407.8 / 2.22	9038	35.0	2.5	<5
3	151	1.77	–36.1	129.1 / 0.83	8055	26.4	4.5	28
DDNP	142	1.76	–45.7	134.2 / 0.63	7290	23.7	1[20]	5[20]
$Pb(N_3)_2$	315	4.80	–11.0	450.1 / 1.54	5876	33.4	2.5–4.0	0.1–1

[a] Decomposition temperature (onset, heating rate: 5 °C/min). [b] Recalculated from low-temperature X-ray densities, $\rho_{298K}=\rho_T/(1+\alpha_v(298-T_0))$ $\alpha_v=1.5\times10^{-4}$, T_0 is the crystal testing temperature. [c] Oxygen balance, for $C_aH_bO_cN_d$: 1600(c-2a-b/2)/M_W, MW= molecular weight. [d] Heat of formation. [e] Detonation velocity (calculated with Explo5 v.6.01) [f] Detonation pressure (calculated with Explo5 v.6.01) [g] Impact sensitivity. [h] Friction sensitivity.

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and **2** are more sensitive than **3**, which can be rationalized by ESP and hydrogen-bond interactions; the more uniform charge distribution (see Figure 6)[37, 38] and the intermolecular hydrogen bonds (as shown in Figure 5) for compound 3 lower its sensitivity.

Conclusions

Three inner diazonium salts, 3,5-dichloro-4-diazopyrazole zwitterion (**1**), 4-diazo-3,5-dinitropyrazole zwitterion (**2**) and 4-diazo-5-nitro-pyrazol-3-one zwitterion (**3**), were successfully synthesized and detailedly characterized. The DSC results that they all have moderately high thermal stabilities though as diazonium salts. The decomposition temperatures of compounds **2** and **3** are 154 °C and 151 °C respectively, which are slightly higher than that of DDNP (T_d= 142°C). In addition, they possess high densities and excellent detonation properties (**2**, 1.81 g cm^{-3}, 9038 m s^{-1}, 35.0 GPa; **3**, 1.77 g cm^{-3}, 8055 m s^{-1}, 26.4 GPa) compared to DDNP (1.76 g cm^{-3}, 7290 m s^{-1}, 23.7 GPa). Based on their reasonable thermal stabilities, high densities, remarkable detonation performances, and high sensitivities, compound **2** and **3** can serve as potential candidates for green primary explosives.

Experimental

Caution : We have synthesized all compounds in millimolar amounts and have experienced no difficulties in their synthesis; however, an explosion took place during the sample grinding process in the IR characterization of **2**, therefore, compound **2** must not be ground. Appropriate protective measures must be used and caution should be exercised at all times during synthesis, characterization and handling of these materials. The use of appropriate safety precautions (safety shields, face shields, leather gloves, protective clothing, such as heavy leather welding suits and ear plugs) is mandatory. Any synthesis of these energetic compounds must be carried out only in small amounts.

General methods

All materials were commercially available and used as received. FT-IR spectra were recorded using KBr pellets for solids on a Bruker Tensor 27 spectrometer. UV/Vis spectra were recorded on a SHIMADZU UV-2600 spectrophotometer. ^{13}C NMR spectra were recorded on a Bruker AM-400 MHz spectrometer (Zurich, Switzerland) operating at 100 MHz with Acetone-d6 as the locking solvent. Chemical shifts are reported in ppm relative to TMS. Electrospray ionization mass spectrum (ESI-MS) was performed on a Bruker APEXII FT-ICR MS instrument (Billerica, MA, USA). MS-EI spectra were recorded on a GCTMS Micromass UK spectrometer. Elemental analyses were performed on an Elementar Vario EL analyzer (Bremen, Germany). DSC studies were carried out on a TA-DSC Q2000 thermal analyzer (New Castle, DE, USA). Detonation pressures and velocities were predicted based on the traditional Chapman-Jouget thermodynamic detonation theory using EXPLO 6.01. Computations were performed using the Gaussian 09 software package. The B3LYP/6-311G++ (d, p) method was used to optimize the molecular structures and calculate the heats of formation and electrostatic potential for these energetic inner diazonium salts. All of the optimized structures were characterized to be true local energy minima on the potential energy surfaces without imaginary frequencies.

Synthesis of LLM-116

This compound was prepared according to a literature method.[25]

Synthesis of 1

LLM-116 (2.5 g, 14.45 mmol) and $KMnO_4$(2.28 g, 14.45 mmol) were successively added to a 36% hydrochloric acid (30 ml) solution, which was heated to 50-60 °C. The mixture was stirred at that temperature for 2 h, and then neutralized by adding a $NaHCO_3$ solution. The mixture was extracted with ethyl acetate and dried over magnesium sulfate; the solvent was then removed under reduced pressure and the product was isolated with satisfactory purity as a brownish yellow solid (1.3 g, 55.2% yield). m/z (ESI-MS) 163 $(M+H)^+$.^{13}C NMR (100 MHz, Acetone-d_6): δ=80.5, 143.5 ppm; ^{15}N NMR (61 MHz, Acetone-d_6): δ = –18.17, –40.35, –146.47 ppm; IR: ν = 2169 (vs),1415 (vs), 1396 (vs), 1373 (m), 1253 (w), 1221 (w), 941 (s), 663 (w), 642 (w), 619 (w); elemental analysis (%) calcd for $C_3Cl_2N_4$: C, 22.11; Cl, 43.51; N, 34.38; found: C 21.90, N 34.11.

Synthesis of 2

LLM-116 (2g, 11.56 mmol), $NaNO_2$(0.8 g, 11.56 mmol) were successively added to a 20% sulfuric acid (20 ml) solution. The reaction mixture was stirred at 0-5°C for 1 h, and subsequently neutralized by adding a $NaHCO_3$ solution. The obtained yellow precipitate was filtered, washed with water, and dried in air (1.06 g, 50% yield). m/z (EI-MS) 184 $(M)^+$; ^{13}C NMR (100 MHz, Acetone-d_6): δ = 76.6, 157.2 ppm; ^{15}N NMR (61 MHz, Acetone-d_6): δ = –28.46, –40.62, –46.24, –156.35 ppm; ppm IR: ν = 2233 (vs),1557 (vs), 1515 (m), 1490 (vs), 1396 (m), 1347 (s), 1320 (s), 835 (s), 643 (w), 591 (w); elemental analysis (%) calcd for $C_3N_6O_4$: C 19.58, N 45.66; found: C 20.29, N 45.34.

Synthesis of 3

Compound **2** (1 g, 5.4 mmol) was added to a 20% sulfuric acid (30 ml), which was heated to 60-70 °C, then the mixture was stirred at that temperature for 2h. The reaction mixture was extracted with ethyl acetate and dried over magnesium sulfate. The solvent was then removed under reduced pressure and the product was isolated with satisfactory purity as a yellow solid (0.6 g, 71.7% yield). m/z (EI-MS) 155 $(M)^+$; ^{13}C NMR (100 MHz, Acetone-d_6): δ = 104.5, 164.1, 174.7 ppm; ^{15}N NMR (61 MHz, Acetone-d$_6$): δ = –8.41, –26.67, –81.69, –135.79, –199.45 ppm; IR: ν = 3212 (m), 2171 (s), 1675 (vs), 1554 (m), 1519 (s), 1462 (m), 1357 (s), 1292 (m), 1183 (m), 1100 (w), 1027 (w), 829 (m), 774 (m), 709 (m), 623 (w), 506 (w); elemental analysis (%) calcd for $C_3HN_5O_3$: C 23.24, H 0.65, N 45.16; found: C 23.66, H 0.85, N 44.53.

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Notes and references

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Synthesis and characterization of three pyrazolate inner diazonium salts: green, powerful and stable primary explosives

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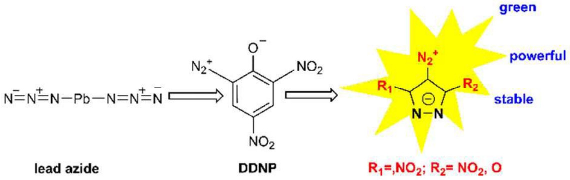

Three pyrazole based inner diazonium salts were synthesized with admirable performances, which can be used as potential primary explosives.