Dalton Transactions

ROYAL SOCIETY OF CHEMISTRY

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Cite this: *Dalton Trans.*, 2024, **53**, 7100

Azidomethyl-bisoxadiazol-linked-1,2,3-triazole-(ABT)-based potential liquid propellant and energetic plasticizer†

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Received 2nd March 2024,
Accepted 25th March 2024

DOI: 10.1039/d4dt00638k

rsc.li/dalton

A scalable synthesis of azidomethyl bisoxadiazol linked-1,2,3-triazole-(ABT) based potential liquid propellant and energetic plasticizer is obtained from commercially available diaminomaleonitrile in excellent yield. Newly synthesized compounds were fully characterized by various spectroscopic techniques. These materials exhibit good densities (1.77 g cm^{-3}) and high thermal stabilities (T_d = 181 °C). Compound **5** has good detonation properties (**5**, P = 20.81 GPa, D = 7516 ms^{-1}) and propulsive properties (I_{sp} (neat) = 210 s). These are superior to TNT and GAP and comparable to BAMOD, making them potential green liquid rocket propellants and energetic plasticizers.

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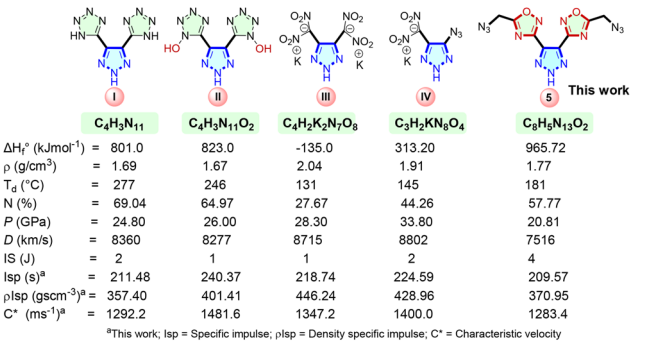
Polyazido heterocycles have been studied extensively due to their wide range of medical, pharmaceutical, and material science applications.[1–5] The azide moiety, a well-known precursor in 3 + 2 cycloadditions and well known in the field of high energy density materials as one of the explosophoric groups ($-N_3$, $-NO_2$, $-ONO_2$, $-NHNO_2$, *etc.*), used to improve the nitrogen content, and heats of formation of these materials.[6] These compounds produce green gaseous products (N_2, N_2O, HN_3, NO_x, *etc.*) during their combustion and deflagration.[7] Polyazido compounds are utilized in various forms, such as energetic polymers, plasticizers, explosives, pyrotechnics, melt castable explosives, and hypergolic liquids.[8] Recently a few heterocycles with the azidomethyl moiety with eminent properties have also been reported.[9,10] 1,2,3-Oxadiazole-derived energetic materials are popular because of their facile syntheses, readily available precursors, and high reaction yields, which help lower the total production cost of the newly designed materials. However, the stabilities and sensitivities of these molecules are a big concern. Therefore, the scientific community is continually working to develop high-performance and less sensitive energetic materials by structural modification or design of new skeletons. Isoxazole and 1,2,4-oxadiazole skeletons with appropriate explosophoric groups could be good choices to design new energetic materials because of the balance between energy and stability. Recently, several 1,2,3-triazole-based energetic compounds namely 4,5-di(1*H*-tetrazol-5-yl)-2*H*-1,2,3-triazole(**I**, **H3BTT**),[11] 4,5-bis(1-hydroxytetrazol-5-yl)-2*H*-1,2,3-triazoledihydrate (**II**, **BHTT**),[11] dipotassium 4,5-bis(dinitromethyl)-2*H*-1,2,3-triazole (**III**, **K_2BDNMT**),[12] potassium-4-azido-5-(dinitromethyl)-2*H*-1,2,3-triazole (**IV**, **KAzDNMT**),[13] 4,5-bis(azidomethyl)-2-nitro-2*H*-1,2,3-triazole (**V**, **BAzMNT**)[14] and (2-nitro-2*H*-1,2,3-triazole-4,5-diyl)bis (methylene) dinitrate (**VI**, **BMDNNT**)[14] have been developed (Fig. 1).

These compounds are highly mechanically sensitive materials (**H3BTT**: IS = 2J, **BHTT**: 1S = 1J, **K_2BDNMT**: IS = 1J, **KAzDNMT**: IS = 2J, **BAzMNT**: IS = 1J, **BMDNNT**: IS = 1J), making them competitive candidates as green primary explosives. 5,5′-Bis(azidomethyl)-3,3′-bi(1,2,4-oxadiazole)[9] exhibits good thermal stability (T_d = 209 °C) and low impact sensitivity (IS = 40 J), which is a good secondary explosive candidate. Due to their high nitrogen content, **H3BTT**, **BHTT** and **BAzMNT** may well be erosion-reduced gun propellant ingredients or gas generators.



	$C_4H_3N_{11}$	$C_4H_3N_{11}O_2$	$C_4H_2K_2N_7O_8$	$C_3H_2KN_8O_4$	$C_8H_5N_{13}O_2$
$\Delta H_f°$ (kJmol^{-1})	801.0	823.0	-135.0	313.20	965.72
ρ (g/cm^3)	1.69	1.67	2.04	1.91	1.77
T_d (°C)	277	246	131	145	181
N (%)	69.04	64.97	27.67	44.26	57.77
P (GPa)	24.80	26.00	28.30	33.80	20.81
D (km/s)	8360	8277	8715	8802	7516
IS (J)	2	1	1	2	4
Isp (s)[a]	211.48	240.37	218.74	224.59	209.57
ρIsp (gscm^{-3})[a]	357.40	401.41	446.24	428.96	370.95
C* (ms^{-1})[a]	1292.2	1481.6	1347.2	1400.0	1283.4

[a]This work; Isp = Specific impulse; ρIsp = Density specific impulse; C* = Characteristic velocity

Fig. 1 Recently developed 1,2,3-triazoles[11–13] and this work.

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†Electronic supplementary information (ESI) available. CCDC 2330491. For ESI and crystallographic data in CIF or other electronic format see DOI: https://doi.org/10.1039/d4dt00638k

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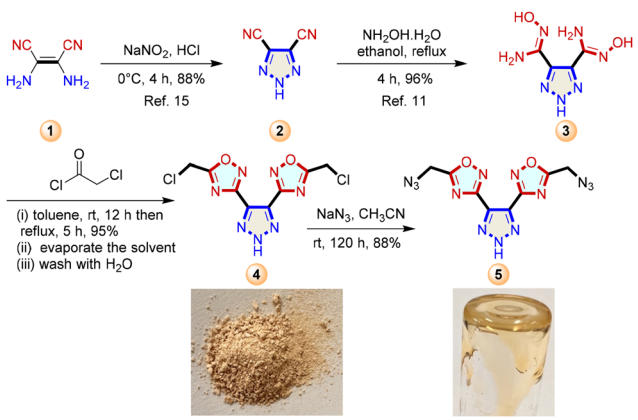
Now we report a unique combination of 1,2,4-oxadiazole and 1,2,3-triazole with azidomethyl functionalities to generate a potential liquid rocket propellants and energetic plasticizer with a better energetic performance and low sensitivity. The preparation of bisamidaoxime **3** is based on the literature procedure.[11,15] Subsequently, compound **3** was treated with chloroacetyl chloride in refluxing toluene to give 4,5-bis(5-(chloromethyl)-1,2,4-oxadiazol-3-yl)-2*H*-1,2,3-triazole (**4**, **BCMODAT**) in excellent yield. Later compound **4**, on treatment with NaN_3, gave 4,5-bis(5-(azidomethyl)-1,2,4-oxadiazol-3-yl)-2*H*-1,2,3-triazole (**5**, **AzM-BOLT**) in excellent yield *via* a sluggish reaction (Scheme 1).

Compound **4** is solid at room temperature while compound **5** is liquid at room temperature. Their thermal stabilities were determined using differential scanning calorimetry (DSC) at the heating rate of 5 °C min^{-1}, (ESI, Fig. S13–S16†). Remarkably, compounds **5** exhibit high thermal stability (T_d = 181 °C).

Compound **4·DMSO** was crystallized by slow recrystallization in DMSO (Fig. 2). The crystal density of compound **4·DMSO** is 1.635 g cm^{-3} at 100 K with single formula unit in the asymmetric unit (Z = 4, Z' = 0.5), and orthorhombic *Pnma* space group as listed in Fig. S2–S5 (see ESI†).

The heats of formation (ΔH_f° (s)) of the newly synthesized compounds were calculated using the isodesmic method (Fig. S1†) with the Gaussian 03 suite of programs.[16] Subsequently, their corresponding detonation and propulsive performance were estimated using (ΔH_f° (s)) and room temperature densities with the help of EXPLO5 V7.01 software.[17] Compound **5** exhibits a very high positive enthalpy of formation (ΔH_f° (s)), 1010.21 kJ mol^{-1} which are superior to CL-20 (ΔH_f° (s) = 608.70 kJ mol^{-1}). Optimized structure, Mulliken and NBO charges of compound **5** are illustrated in Fig. 3 and 4 respectively.

Additionally, a detailed study on the detonation and propulsive performance was carried out for the new materials shows that compound **5** has good potential as liquid rocket propellant and energetic plasticizer. Composite propellants (with AP/Al/HTPB) performed slightly lower than those of individual neat mono-propellant compounds. Whereas, the performance of the new compounds was notably better with aluminium (Al) as a fuel additive.



Scheme 1 Synthesis of compounds **4** and **5**.

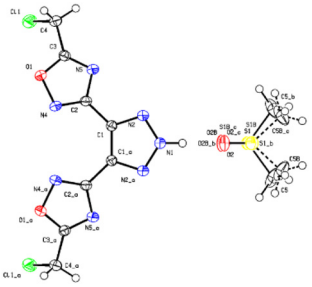


Fig. 2 Single crystal X-ray structure of compound **4·DMSO** (CCDC 2330491†).

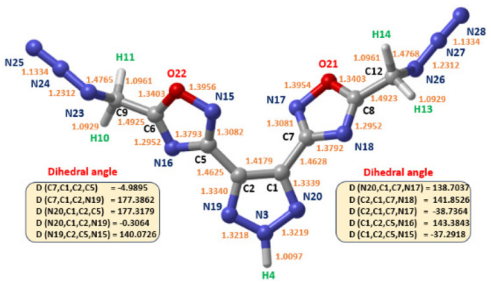


Fig. 3 Optimized structure of **5** obtained using the B3LYP/6-311++G(d,p) level of theory.

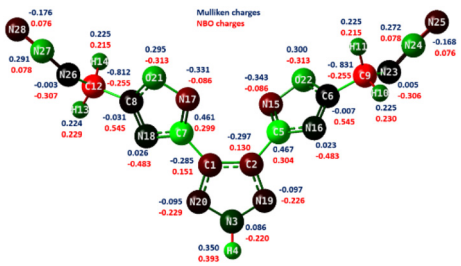


Fig. 4 Mulliken and NBO charges of compound **5**.

The weak interactions between the oxadiazole rings and the presence of spacer ($-CH_2$) provided additional stability to compound **5**. The ESP maxima and minima for compound **5** are 60.09 kcal mol^{-1} and −28.65 kcal mol^{-1}, respectively (Fig. 5).

Furthermore, several non-covalent interactions and reduced density gradients were determined in compound **5** using B3LYP/6-311++G(d,p) level of theory (Fig. 6). This shows that compound **5** has good numbers of weak interactions (VDW and H-bonding) and corporately less steric effects, resulting in high thermal stability.

Additionally, the bond dissociation energy (BDE, gas-phase) of homolytic cleavage of the $-CH_2-N_3$ $-N_2$ and $-N_3$ bonds were predicted at B3LYP/6-311++G(d,p) level of theory. Compound **5** exhibits high BDEs 330.24 kJ mol^{-1} ($-CH_2-N_3$);

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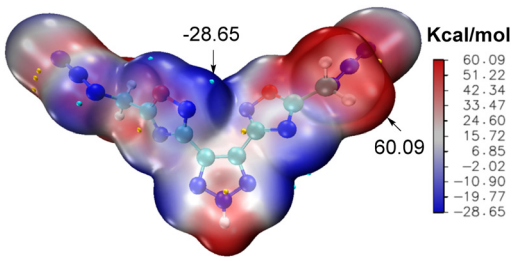

Fig. 5 Electrostatic potential maps of compound **5**.

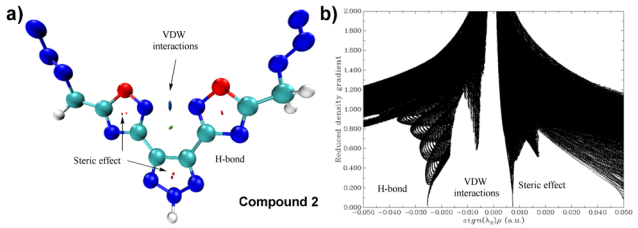

Fig. 6 Non-covalent interaction (NCI): (a) reduced density gradient (RDG) and (b) scatter diagram of compound **5**.

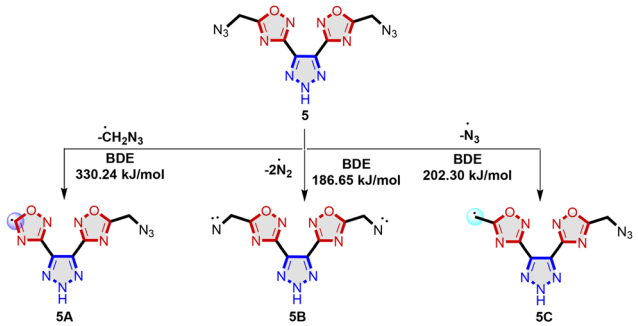

Fig. 7 Bond dissociation energies of compound **5**.

186.65 kJ mol^{-1} ($-N_2$) and 202.3 kJ mol^{-1} ($-N_3$), supports it high thermal stability (Fig. 7).

The detonation performance of compound **5** was calculated using its solid-phase heats of formation and experimental densities with EXPLO5 V 7.01 program[17] and results are given in Table 1. Compound **5** (P = 20.81 GPa, D = 7516 ms^{-1}, Q = 3925 kJ kg^{-1}), which are comparable to those of compound BAMOD (P = 22.70 GPa, D = 7672 ms^{-1}, Q = 4724 kJ kg^{-1}) and superior to TNT (P = 18.56 GPa, D = 6839 ms^{-1}, Q = 4395 kJ kg^{-1}).

In summary, a facile synthesis of compound **5** from commercially available diaminomaleonitrile (DAMN) was developed. The newly synthesized compounds were fully characterized by FTIR, NMR, and elemental analyses. A detailed study of energetic performance and thermal behaviour of compound **5** was also carried out. Compound **5** possess high thermal stabilities (T_d, 181 °C) and low sensitivities toward friction (120 N) and impact (4 J). Compound **5** (P = 20.81 GPa, D = 7516 ms^{-1}, I_{sp} = 210 s), has potential as a liquid propellant and energetic plasticizer in rocket propulsion.

Table 1 Comparison of physicochemical properties

Compound	**5**	GAP[a]	BAMOD[b]	TNT[c]
Formula[d]	$C_8H_5N_{13}O_2$	$C_3H_5N_3O$	$C_8H_4N_{12}O_3$	$C_7H_5N_3O_6$
FW [g mol^{-1}][e]	315.21	—	316.21	227.13
OB^{CO} (%)[f]	−43.15	−72.66	−35.42	−24.66
OB^{CO_2} (%)[g]	−83.75	−121.10	−75.90	−73.97
N + O [%][h]	67.92	16.15	68.34	60.76
N [%][i]	57.77	42.41	53.16	18.50
ΔH_f [kJ mol^{-1}][j]	1010.21	141.94	1072.90	70.30
ρ [g cm^{-3}][k]	1.77	1.29	1.75	1.65
T_d [°C][l]	181	−45	193	300
D [ms^{-1}][m]	7516	6303	7672	6839
P [GPa][n]	20.81	15.41	22.70	18.56
$-Q$ [kJ kg^{-1}][o]	3925	3635	4724	4395
M[g mol^{-1}][p]	27.78	32.07	27.65	26.47
IS [J][q]	4	9	—	15
FS [N][r,x]	120	444	80	353
I_{sp} [s][s,x]	209.57	198.46	229.17[y]	206.49[y]
ρI_{sp} [s][t,x]	370.95	256.60	401.05[y]	341.54[y]
C^* [ms^{-1}][u,x]	1283.4	1207.8	1399.5[y]	1283.5[y]
I_{sp} [s][v,x]	217.84	224.79	231.56[y]	232.00[y]
I_{sp} [s][w,x]	207.56	218.97	220.78[y]	225.11[y]

[a] Ref. 17. [b] Ref. 9. [c] Ref. 17. [d] Molecular formula. [e] Molecular weight. [f] CO based oxygen balance. [g] CO_2 based oxygen balance. [h] N + O contents in %. [i] Nitrogen content in %. [j] Calculated enthalpy of formation. [k] Measured densities, gas pycnometer at room temperature. [l] Melting point and decomposition temperature (onset) under nitrogen gas (DSC, 5 °C min^{-1}). [m] Calculated detonation velocity. [n] Calculated detonation pressure. [o] Heat of detonation. [p] Mole of gaseous products. [q] Measured impact sensitivity (IS). [r] Measured friction sensitivity (FS). [s] I_{sp} = Specific impulse of neat compound (monopropellant). [t] ρI_{sp} = Density specific impulse of neat compound (monopropellant). [u] Characteristic velocity. [v] I_{sp} = Specific impulse at 88% compound and 12% Al. [w] I_{sp} = Specific impulse at 78% compound, 12% Al (fuel additive) and 10% binder (HTPB). [x] Specific impulse calculated at an isobaric pressure of 70 bar and initial temperature of 3300 K using EXPLO5 V 7.01. [y] This work.

Experimental section

Compounds **2** [15] and **3** [11] were prepared according to literature procedure (see ESI†).

4,5-Bis(5-(chloromethyl)-1,2,4-oxadiazol-3-yl)-2*H*-1,2,3-triazole (4)

Compound **3** (2.590 g, 14 mmol, 1.0 equiv.) was dissolved in toluene (10 mL), and the resulting mixture was cooled to 0 °C. Then chloroacetyl chloride (5.53 g, 3.9 mL, 49 mmol, 3.5 equiv.) was added dropwise. The resulting reaction mixture was stirred at room temperature for 12 h and was subsequently refluxed for 6 h. After cooling to room temperature, the solvent was evaporated under reduced pressure, and the crude product was washed with water (5 × 20 mL), precipitate was collected by filtration, which was further recrystallized from ethanol. Crystalline, brown solid; yield: 4.0 g, 95%, DSC (5 °C min^{-1}): T_m (onset) 71 °C, T_d (onset) 316 °C; IR (KBr pellet) υ 3615 (s), 3354 (s), 3186 (s), 2948 (s), 2806 (s), 2745 (s), 2626 (m), 1625 (s), 1581 (s), 1427 (s), 1397 (s), 1370 (m), 1319 (w), 1270 (m), 1237 (m), 1205 (m), 1096 (s), 1022 (w), 996 (s), 952 (s), 907 (s), 892 (s), 860 (m), 790 (s), 732 (m), 641 (w), 489 (w) cm^{-1}; ^{1}H NMR (500.19 MHz, DMSO-d_6): δ 5.20 (s, 4H), 16.61 (s, 1H); ^{13}C NMR (125.8 MHz, DMSO-d_6): δ 33.7, 133.2, 161.4,

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176.1; elemental analysis: calcd (%) for $C_8H_5Cl_2N_7O_2$ (302.08): C, 31.8; H, 1.67; N, 32.46. Found C, 31.90; H, 1.80; N, 32.37.

4,5-Bis(5-(azidomethyl)-1,2,4-oxadiazol-3-yl)-2*H*-1,2,3-triazole (5)

Compound **4** (2.416 g, 8.0 mmol, 1.0 equiv.) was dissolved in acetonitrile (20 mL), and sodium azide (2.080 g, 32.00 mmol, 4.0 equiv.) was added. The resulting mixture was stirred at room temperature for 120 h. Then, the solid was filtered and washed with (5 × 20 mL) of acetonitrile. The filtrate was dried over anhydrous Na_2SO_4 and the solvent was evaporated under reduced pressure at room temperature. The resulting crude material was further purified by flash column chromatography or trituration. Yellow viscous liquid; Yield: 2.21 g, 88%, DSC (5 °C min^{-1}): T_d (onset) 181 °C; IR (KBr pellet) υ 3211 (s), 2965 (s), 2920 (s), 2847 (s), 2107 (s), 1581 (s), 1429 (s), 1326 (s), 1247 (s), 1247 (s), 1200 (s), 1097 (s), 1019 (m), 990 (m), 953 (s), 901 (s), 767 (s), 742 (s), 671 (m), 555 (m) cm^{-1}; ^1H NMR (500.19 MHz, DMSO-d_6): δ 4.98 (s, 4H); ^{13}C NMR (125.77 MHz, DMSO-d_6): δ 44.5, 132.8, 161.7, 175.6; elemental analysis: calcd (%) for $C_8H_5N_{13}O_2{\cdot}0.6H_2O$ (326.03): C, 29.47; H, 1.92; N, 55.85. Found C, 29.79; H, 1.94; N, 55.51.

Author contributions

S. L. investigation, methodology, conceptualization and manuscript writing. R. J. S. X-ray data collection and structure solving. S. L. and J. M. S. conceptualization, manuscript writing-review and editing, supervision.

Conflicts of interest

The authors declare no competing financial interest.

Acknowledgements

The Rigaku Synergy S Diffractometer was purchased with support from the National Science Foundation MRI program (1919565). We are grateful for the support of the Fluorine-19 fund.

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