Supporting Information

Synthesis, single crystal structure of fully-substituted polynitrobenzene derivatives for high-energy materials

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Spectral data of 8
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Crystal structures and crystalline parameters

Fig. S1 (a) Thermal ellipsoid plot (50%) and labelling scheme of 6. (b) Ball-and-stick packing diagram of 6 viewed down the a axis. Dashed lines indicate strong hydrogen bonding.
Fig. S2 (a) Thermal ellipsoid plot (50%) and labelling scheme of 7. (b) Ball-and-stick packing diagram of 7 viewed down the $b$ axis. Dashed lines indicate strong hydrogen bonding.
Fig. S3 Figure showing the nitro-π interactions (dashed red lines between nitro oxygen atoms and ring centroids) for each molecule of 7
Fig. S4 (a) Thermal ellipsoid plot (50%) and labelling scheme of 8. (b) Ball-and-stick packing diagram of 8 viewed down the $a$ axis. Dashed lines indicate strong hydrogen bonding.
Table S1. Crystal data and structure refinement details for 4, 5, 6, 7 and 8

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Table S2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for 4. U(eq) is defined as one third of the trace of the orthogonalized U̅ tensor.

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Table S3. Bond lengths [Å] and angles [°] for 4.

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C(13)-C(14)-N(10) 119.5(2)
N(8)-C(15)-N(6) 111.0(2)
N(8)-C(15)-C(16) 39.34(15)
N(6)-C(15)-C(16) 71.69(16)
N(8)-C(15)-H(15) 124.5
N(6)-C(15)-H(15) 124.5
C(16)-C(15)-H(15) 163.8
N(7)-C(16)-N(8) 116.2(2)
N(7)-C(16)-C(15) 77.83(17)
N(8)-C(16)-C(15) 38.38(13)
N(7)-C(16)-H(16) 121.9
N(8)-C(16)-H(16) 121.9
C(15)-C(16)-H(16) 160.3

Symmetry transformations used to generate equivalent atoms:

Table S4.  Anisotropic displacement parameters (Å² x 10³) for 4. The anisotropic displacement factor exponent takes the form: \( -2p^2 [ h^2 a^* u^{11} + \ldots + 2h k a^* b^* u^{12} ] \).

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Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for 4.

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Table S6. Torsion angles [°] for 4.
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C(1)-C(1)-C(2)-C(3) 179.73(17)
C(6)-C(1)-C(2)-N(1) 177.2(2)
C(1)-C(1)-C(2)-N(1) -2.3(3)
Cl(1)-C(1)-C(2)-C(3) 179.73(17)
Cl(1)-C(1)-C(2)-N(1) -2.3(3)
C(7)-N(1)-C(2)-C(3) -177.7(2)
C(7)-N(1)-C(2)-C(1) 87.8(3)
N(2)-N(1)-C(2)-C(3) 99.1(3)
C(7)-N(1)-C(2)-C(1) 90.1(3)
N(2)-N(1)-C(2)-C(3) -83.0(3)
C(1)-C(1)-C(2)-C(3) 0.2(3)
N(1)-C(2)-C(3)-N(4) -177.7(2)
C(1)-C(2)-C(3)-Cl(2) 177.97(17)
N(1)-C(2)-C(3)-Cl(2) 0.0(3)
C(2)-C(3)-C(4)-C(5) 0.6(3)
Cl(2)-C(3)-C(4)-C(5) -177.12(17)
C(2)-C(3)-C(4)-N(4) -179.1(2)
C(1)-C(2)-C(3)-C(4) 3.1(3)
O(1)-N(4)-C(4)-C(3) 86.1(3)
O(2)-N(4)-C(4)-C(3) -91.9(3)
O(1)-N(4)-C(4)-C(5) -93.7(3)
O(2)-N(4)-C(4)-C(5) 88.4(3)
C(3)-C(4)-C(5)-C(6) -1.0(3)
N(4)-C(4)-C(5)-C(6) 178.8(2)
C(3)-C(4)-C(5)-Cl(3) -179.28(18)
N(4)-C(4)-C(5)-Cl(3) 0.5(3)
C(4)-C(5)-C(6)-C(1) 0.5(3)
Cl(3)-C(5)-C(6)-C(1) 178.78(18)
C(4)-C(5)-C(6)-N(5) -178.4(2)
C(3)-C(5)-C(6)-N(5) -0.1(3)
C(2)-C(1)-C(6)-C(5) 0.3(3)
Cl(1)-C(1)-C(6)-C(5) 179.89(18)
C(2)-C(1)-C(6)-N(5) 179.2(2)
Cl(1)-C(1)-C(6)-N(5) -1.3(3)
O(4)-N(5)-C(6)-C(5) 101.7(3)
O(4)-N(5)-C(6)-C(1) 103.4(3)
O(3)-N(5)-C(6)-C(1) -77.2(3)
C(8)-N(3)-C(7)-N(1) -0.3(3)
N(2)-N(1)-C(7)-N(3) 0.0(3)
C(2)-N(1)-C(7)-N(3) -173.8(2)
N(2)-N(1)-C(7)-C(8) -0.2(2)
C(2)-N(1)-C(7)-C(8) -174.0(2)
N(1)-N(2)-C(8)-N(3) -0.5(4)
N(1)-N(2)-C(8)-C(7) -0.20(19)
C(7)-N(3)-C(8)-N(2) 0.5(4)
C(14)-C(9)-C(10)-C(11) -0.5(3)
Cl(4)-C(9)-C(10)-N(9) 178.1(2)
Cl(4)-C(9)-C(10)-N(9) -0.1(3)
O(5)-N(9)-C(10)-C(9) -94.1(3)
O(6)-N(9)-C(10)-C(9) 86.6(3)
O(5)-N(9)-C(10)-C(11) 84.6(3)
O(6)-N(9)-C(10)-C(11) -94.8(3)
C(9)-C(10)-C(11)-C(12) -1.6(3)
N(9)-C(10)-C(11)-C(12) 179.7(2)
C(9)-C(10)-C(11)-Cl(5) -179.60(18)
N(9)-C(10)-C(11)-Cl(5) 1.8(3)
C(10)-C(11)-C(12)-C(13) 2.8(3)
Cl(5)-C(11)-C(12)-C(13) -179.26(17)
C(10)-C(11)-C(12)-N(6) -176.3(2)
Cl(5)-C(11)-C(12)-N(6) 1.6(3)
C(15)-N(6)-C(12)-C(13) -88.8(3)
N(7)-N(6)-C(12)-C(13) 86.0(3)
C(15)-N(6)-C(12)-C(11) 90.3(3)
N(7)-N(6)-C(12)-C(11) -94.9(3)
C(11)-C(12)-C(13)-C(14) -1.7(3)
N(6)-C(12)-C(13)-C(14) 177.3(2)
C(11)-C(12)-C(13)-Cl(6) -179.33(17)
N(6)-C(12)-C(13)-Cl(6) -0.2(3)
C(10)-C(9)-C(14)-C(13) 1.6(3)
Cl(4)-C(9)-C(14)-C(13) 179.74(18)
C(10)-C(9)-C(14)-N(10) -176.6(2)
Cl(4)-C(9)-C(14)-N(10) 1.5(3)
C(12)-C(13)-C(14)-C(9) -0.4(3)
Cl(6)-C(13)-C(14)-C(9) 177.11(18)
C(12)-C(13)-C(14)-N(10) 177.8(2)
Cl(6)-C(13)-C(14)-N(10) -4.7(3)
O(7)-N(10)-C(14)-C(9) -73.5(3)
O(8)-N(10)-C(14)-C(9) 105.7(3)
O(7)-N(10)-C(14)-C(13) 108.2(3)
O(8)-N(10)-C(14)-C(13) -72.5(3)
C(16)-N(8)-C(15)-N(6) 0.7(3)
N(7)-N(6)-C(15)-N(8) -0.9(3)
C(12)-N(6)-C(15)-N(8) 174.5(2)
N(7)-N(6)-C(15)-C(16) -0.40(19)
C(12)-N(6)-C(15)-C(16) 174.9(2)
N(6)-N(7)-C(16)-N(8) -0.2(3)
O(1)-N(7)-C(16)-N(8) 118.3(2)
O(1)-N(7)-C(16)-C(15) 118.10(13)
C(15)-N(8)-C(16)-N(7) -0.3(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z  #2 x+1/2,-y+1/2,z-1/2  #3 -x+1,-y,-z
#4 x-1/2,-y+1/2,z+1/2

Table S7. Hydrogen bonds for 4 [Å and °].

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Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z  #2 x+1/2,-y+1/2,z-1/2  #3 -x+1,-y,-z
#4 x-1/2,-y+1/2,z+1/2

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å² x 10^3) for 5.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

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Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters (Å²x 10³) for 5. The anisotropic displacement factor exponent takes the form: -2π² [ h²a²U₁₁ + ... + 2hka*b*U₁₂ ]

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**Table S11.** Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 5.
Table S12. Torsion angles ['] for 5.

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O(8)-N(10)-C(14)-C(13) 93.7(7)
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C(13)-C(14)-C(15)-N(11) -178.8(4)
N(10)-C(14)-C(15)-N(11) -0.2(7)
N(12)-N(11)-C(15)-C(14) -106.3(7)
C(19)-N(11)-C(15)-C(14) 79.6(8)
C(19)-N(11)-C(15)-C(16) -100.0(7)
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C(14)-C(15)-C(16)-N(14) -174.3(4)
N(11)-C(15)-C(16)-N(14) 5.3(7)
N(12)-C(11)-C(16)-C(15) -2.5(7)
Cl(3)-C(11)-C(16)-C(15) -179.1(4)
C(12)-C(11)-C(16)-N(14) 173.1(4)
Cl(3)-C(11)-C(16)-N(14) -3.6(6)
C(17)-N(14)-C(16)-C(15) -118.5(7)
N(15)-N(14)-C(16)-C(15) 62.4(7)
N(15)-N(14)-C(16)-C(11) -113.2(6)
N(15)-N(14)-C(16)-C(11) -113.2(6)
N(15)-N(14)-C(16)-N(14) 6.4(7)
N(15)-N(14)-C(16)-N(14) 6.4(7)
N(15)-N(14)-C(17)-N(16) 1.1(8)
C(16)-N(14)-C(17)-N(16) -178.1(6)
N(14)-N(15)-C(18)-N(16) 0.9(10)
C(17)-N(16)-C(18)-N(15) -0.3(11)
C(20)-N(13)-C(19)-N(11) 3.7(9)
N(12)-N(11)-C(19)-N(13) -3.6(9)
C(15)-N(11)-C(19)-N(13) 171.1(6)
N(12)-N(11)-C(19)-C(20) -1.1(6)
C(15)-N(11)-C(19)-C(20) 173.6(6)
N(11)-N(12)-C(20)-N(13) 0.7(10)
N(11)-N(12)-C(20)-C(19) -1.1(5)
C(19)-N(13)-C(20)-N(12) -2.8(11)

Symmetry transformations used to generate equivalent atoms:
Table S13. Hydrogen bonds for 5 [Å and °].

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<th>d(H...A)</th>
<th>d(D...A)</th>
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<td>3.202(7)</td>
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Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z+1/2    #2 -x+1,-y+1,-z+1    #3 -x+2,-y+2,-z
#4 x,-y+3/2,z-1/2

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å² x 10^3) for 6. U(eq) is defined as one third of the trace of the orthogonalized U^ij tensor.

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Table S15. Bond lengths [Å] and angles [°] for 6.
N(3)-C(2) 1.329(3)
N(3)-C(3) 1.431(2)
N(4)-C(4) 1.323(3)
N(4)-H(4A) 0.8600
N(4)-H(4B) 0.8600
N(5)-O(1) 1.236(2)
N(5)-O(2) 1.242(2)
N(5)-C(5) 1.404(3)
N(6)-C(6) 1.318(3)
N(6)-H(6A) 0.8600
N(6)-H(6B) 0.8600
N(7)-O(4) 1.240(2)
N(7)-O(3) 1.253(2)
N(7)-C(7) 1.394(3)
N(8)-C(8) 1.325(3)
N(8)-H(8A) 0.8600
N(8)-H(8B) 0.8600
N(9)-C(10) 1.307(3)
N(9)-C(9) 1.352(3)
N(10)-C(9) 1.303(3)
N(10)-N(11) 1.368(2)
N(11)-C(10) 1.329(3)
N(11)-C(11) 1.430(2)
N(12)-C(12) 1.325(3)
N(12)-H(12A) 0.8600
N(12)-H(12B) 0.8600
N(13)-O(5) 1.234(2)
N(13)-O(6) 1.246(2)
N(13)-C(13) 1.408(3)
N(14)-C(14) 1.314(3)
N(14)-H(14A) 0.8600
N(14)-H(14B) 0.8600
N(15)-O(8) 1.238(2)
N(15)-O(7) 1.245(2)
N(15)-C(15) 1.392(3)
N(16)-C(16) 1.325(3)
N(16)-H(16A) 0.8600
N(16)-H(16B) 0.8600
C(1)-H(1A) 0.9300
C(2)-H(2A) 0.9300
C(3)-C(8) 1.390(3)
C(3)-C(4) 1.393(3)
C(4)-C(5) 1.436(3)
C(5)-C(6) 1.431(3)
C(6)-C(7) 1.440(3)
C(7)-C(8) 1.438(3)
C(9)-H(9) 0.9300
C(10)-H(10) 0.9300
C(11)-C(16) 1.388(3)
C(11)-C(12) 1.394(3)
C(12)-C(13) 1.433(3)
C(13)-C(14) 1.432(3)
C(14)-C(15) 1.433(3)
C(15)-C(16) 1.443(3)

C(2)-N(1)-C(1) 101.80(19)
C(1)-N(2)-N(3) 101.54(19)
C(2)-N(3)-N(2) 108.93(18)
C(2)-N(3)-C(3) 129.31(19)
N(2)-N(3)-C(3) 121.75(17)
C(4)-N(4)-H(4A) 120.0
C(4)-N(4)-H(4B) 120.0
H(4A)-N(4)-H(4B) 120.0
O(1)-N(5)-O(2) 117.77(18)
O(1)-N(5)-C(5) 120.82(18)
O(2)-N(5)-C(5) 121.40(19)
C(6)-N(6)-H(6A) 120.0
C(6)-N(6)-H(6B) 120.0
H(6A)-N(6)-H(6B) 120.0
O(4)-N(7)-O(3) 117.33(17)
O(4)-N(7)-C(7) 121.66(17)
O(3)-N(7)-C(7) 121.01(17)
C(8)-N(8)-H(8A) 120.0
C(8)-N(8)-H(8B) 120.0
H(8A)-N(8)-H(8B) 120.0
C(10)-N(9)-C(9) 102.19(18)
C(9)-N(10)-N(11) 101.89(19)
C(10)-N(11)-N(10) 109.01(17)
C(10)-N(11)-C(11) 129.89(18)
N(10)-N(11)-C(11) 121.09(17)
C(12)-N(12)-H(12A) 120.0
C(12)-N(12)-H(12B) 120.0
H(12A)-N(12)-H(12B) 120.0
O(5)-N(13)-O(6) 118.72(17)
O(5)-N(13)-C(13) 121.19(17)
O(6)-N(13)-C(13) 120.08(18)
C(14)-N(14)-H(14A) 120.0
C(14)-N(14)-H(14B) 120.0
H(14A)-N(14)-H(14B) 120.0
O(8)-N(15)-O(7) 117.57(18)
O(8)-N(15)-C(15) 121.55(17)
O(7)-N(15)-C(15) 120.85(17)
C(16)-N(16)-H(16A) 120.0
C(16)-N(16)-H(16B) 120.0
H(16A)-N(16)-H(16B) 120.0
N(2)-C(1)-N(1) 116.2(2)
N(2)-C(1)-H(1A) 121.9
N(1)-C(1)-H(1A) 121.9
N(1)-C(2)-N(3) 111.5(2)
N(1)-C(2)-H(2A) 124.2
N(3)-C(2)-H(2A) 124.2
C(8)-C(3)-C(4) 123.80(18)
C(8)-C(3)-N(3) 118.31(17)
C(4)-C(3)-N(3) 117.78(18)
N(4)-C(4)-C(3) 118.53(19)
N(4)-C(4)-C(5) 123.00(18)
C(3)-C(4)-C(5) 118.47(18)
N(5)-C(5)-C(6) 120.29(19)
N(5)-C(5)-C(4) 119.42(18)
C(6)-C(5)-C(4) 120.27(18)
N(6)-C(6)-C(5) 120.9(2)
N(6)-C(6)-C(7) 120.6(2)
C(5)-C(6)-C(7) 118.52(18)
N(7)-C(7)-C(8) 119.06(17)
N(7)-C(7)-C(6)  120.33(18)
C(8)-C(7)-C(6)  120.58(18)
N(8)-C(8)-C(3)  119.20(19)
N(8)-C(8)-C(7)  122.79(18)
C(3)-C(8)-C(7)  118.01(17)
N(10)-C(9)-N(9)  115.7(2)
N(10)-C(9)-H(9)  122.1
N(9)-C(9)-H(9)  122.1
N(9)-C(10)-N(11)  111.2(2)
N(9)-C(10)-H(10)  124.4
N(11)-C(10)-H(10)  124.4
C(16)-C(11)-C(12)  124.35(18)
C(16)-C(11)-N(11)  117.92(17)
C(12)-C(11)-N(11)  117.69(18)
N(12)-C(12)-C(11)  119.15(18)
N(12)-C(12)-C(13)  122.93(19)
C(11)-C(12)-C(13)  117.90(18)
N(13)-C(13)-C(14)  120.09(17)
N(13)-C(13)-C(12)  119.20(18)
C(14)-C(13)-C(12)  120.67(18)
N(14)-C(14)-C(13)  121.04(19)
N(14)-C(14)-C(15)  120.75(19)
C(13)-C(14)-C(15)  118.21(17)
N(15)-C(15)-C(14)  120.02(17)
N(15)-C(15)-C(16)  119.18(17)
C(14)-C(15)-C(16)  120.80(18)
N(16)-C(16)-C(11)  119.80(18)
N(16)-C(16)-C(15)  122.97(18)
C(11)-C(16)-C(15)  117.23(17)

Symmetry transformations used to generate equivalent atoms:

Table S16. Anisotropic displacement parameters  (Å² x 10³) for 6. The anisotropic displacement factor exponent takes the form: -2π²[ h² a² U₁₁ + ... + 2 h k a* b* U₁₂ ]

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**Table S17.** Hydrogen coordinates (×10^4) and isotropic displacement parameters (Å^2×10^3) for 6.
Table S18. Torsion angles [°] for 6.

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O(1)-N(5)-C(5)-C(4)  -2.6(3)
O(2)-N(5)-C(5)-C(4)  176.4(2)
N(4)-C(4)-C(5)-N(5)  -4.7(3)
C(3)-C(4)-C(5)-N(5)  175.4(2)
N(4)-C(4)-C(5)-C(6)  174.0(2)
C(3)-C(4)-C(5)-C(6)  -6.0(3)
N(5)-C(5)-C(6)-N(6)  0.3(4)
C(4)-C(5)-C(6)-N(6)  -178.3(2)
N(5)-C(5)-C(6)-C(7)  -179.9(2)
C(4)-C(5)-C(6)-C(7)  1.5(3)
O(4)-N(7)-C(7)-C(8)  -1.9(3)
O(3)-N(7)-C(7)-C(6)  177.6(2)
O(4)-N(7)-C(7)-C(6)  176.3(2)
O(3)-N(7)-C(7)-C(6)  -4.3(3)
N(6)-C(6)-C(7)-N(7)  4.6(4)
C(5)-C(6)-C(7)-N(7)  -175.2(2)
N(6)-C(6)-C(7)-C(8)  -177.3(2)
C(5)-C(6)-C(7)-C(8)  3.0(3)
C(4)-C(3)-C(8)-N(8)  177.6(2)
N(3)-C(3)-C(8)-N(8)  1.6(3)
C(4)-C(3)-C(8)-C(7)  -1.9(3)
N(3)-C(3)-C(8)-C(7)  -177.89(18)
N(7)-C(7)-C(8)-N(8)  -4.2(3)
C(6)-C(7)-C(8)-N(8)  177.6(2)
N(7)-C(7)-C(8)-C(3)  175.33(19)
C(6)-C(7)-C(8)-C(3)  -2.9(3)
N(11)-N(10)-C(9)-N(9)  0.1(2)
C(10)-N(9)-C(9)-N(10)  -0.2(3)
C(9)-N(9)-C(10)-N(11)  0.2(2)
N(10)-N(11)-C(10)-N(9)  -0.2(2)
C(11)-N(11)-C(10)-N(9)  -179.06(19)
C(10)-N(11)-C(11)-C(16)  -92.1(3)
N(10)-N(11)-C(11)-C(16)  89.1(2)
C(10)-N(11)-C(11)-C(12)  90.2(3)
N(10)-N(11)-C(11)-C(12)  -88.5(2)
C(16)-C(11)-C(12)-N(12)  -179.9(2)
N(11)-C(11)-C(12)-N(12)  -2.4(3)
C(16)-C(11)-C(12)-C(13)  -1.2(3)
N(11)-C(11)-C(12)-C(13)  176.33(18)
O(5)-N(13)-C(13)-C(14)  168.6(2)
O(6)-N(13)-C(13)-C(14)  -10.9(3)
O(5)-N(13)-C(13)-C(12)  -9.1(3)
O(6)-N(13)-C(13)-C(12)  171.5(2)
N(12)-C(12)-C(13)-N(13)  3.2(3)
C(11)-C(12)-C(13)-N(13)  -175.42(18)
N(12)-C(12)-C(13)-C(14)  -174.4(2)
C(11)-C(12)-C(13)-C(14)  6.9(3)
N(13)-C(13)-C(14)-N(14)  -1.5(3)
C(12)-C(13)-C(14)-N(14)  176.1(2)
N(13)-C(13)-C(14)-C(15)  178.09(19)
C(12)-C(13)-C(14)-C(15)  -4.3(3)
O(8)-N(15)-C(15)-C(14)  173.7(2)
O(7)-N(15)-C(15)-C(14)  -8.0(3)
O(8)-N(15)-C(15)-C(16)  -5.4(3)
O(7)-N(15)-C(15)-C(16)  172.9(2)
N(14)-C(14)-C(15)-N(15)  -3.5(3)
C(13)-C(14)-C(15)-N(15)  176.9(2)
N(14)-C(14)-C(15)-C(16)  175.5(2)
C(13)-C(14)-C(15)-C(16)  -4.0(3)
C(12)-C(11)-C(16)-N(16)  173.9(2)
N(11)-C(11)-C(16)-N(16)  -3.5(3)
C(12)-C(11)-C(16)-C(15)  -6.9(3)
N(11)-C(11)-C(16)-C(15)  175.63(18)
N(15)-C(15)-C(16)-N(16)  7.7(3)
C(14)-C(15)-C(16)-N(16)  -171.4(2)
N(15)-C(15)-C(16)-C(11)  -171.5(2)
C(14)-C(15)-C(16)-C(11)  9.4(3)

Symmetry transformations used to generate equivalent atoms:

Table S19. Hydrogen bonds for 6 [Å and °].

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**Table S20.** Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 7. U(eq) is defined as one third of the trace of the orthogonalized U_ij tensor.

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### Table S21. Bond lengths [Å] and angles [°] for 7.

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[S 45 / S60]

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C(7)-H(7) 0.9300
C(8)-H(8) 0.9300

N(2)-N(1)-C(1) 117.77(18)
N(3)-N(2)-N(1) 170.4(3)
O(1)-N(4)-O(2) 123.7(2)
O(1)-N(4)-C(2) 118.12(18)
O(2)-N(4)-C(2) 118.09(18)
N(6)-N(5)-C(3) 118.71(18)
N(7)-N(6)-N(5) 171.2(2)
O(3)-N(8)-O(4) 125.3(2)
O(3)-N(8)-C(4) 117.7(2)
O(4)-N(8)-C(4) 117.0(2)
N(10)-N(9)-C(5) 117.87(18)
N(11)-N(10)-N(9) 169.8(2)
C(8)-N(12)-N(13) 109.34(17)
C(8)-N(12)-C(6) 129.82(18)
N(13)-N(12)-C(6) 120.83(16)
C(7)-N(13)-N(12) 101.20(19)
C(8)-N(14)-C(7) 102.7(2)
C(6)-C(1)-C(2) 119.38(19)
C(6)-C(1)-N(1) 124.21(19)
C(2)-C(1)-N(1) 116.41(19)
C(3)-C(2)-C(1) 121.42(19)
C(3)-C(2)-N(4) 120.53(18)
C(1)-C(2)-N(4) 118.04(18)
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C(4)-C(3)-N(5) 114.68(19)
C(2)-C(3)-N(5) 128.3(2)
C(5)-C(4)-C(3) 123.40(19)
C(5)-C(4)-N(8) 118.76(18)
C(3)-C(4)-N(8) 117.75(18)
C(4)-C(5)-C(6) 117.89(19)
C(4)-C(5)-N(9) 115.85(18)
C(6)-C(5)-N(9) 126.24(18)
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N(13)-C(7)-H(7) 121.9
N(14)-C(7)-H(7) 121.9
N(14)-C(8)-N(12) 110.6(2)
N(14)-C(8)-H(8) 124.7
N(12)-C(8)-H(8) 124.7

Symmetry transformations used to generate equivalent atoms:

Table S22. Anisotropic displacement parameters (Å² x 10³) for 7. The anisotropic displacement factor exponent takes the form: -2π² | h² a*² U11 + ... + 2 h k a* b* U12 |

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Table S23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^{-3}) for 7.

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Table S24. Torsion angles [°] for 7.

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N(8)-C(4)-C(5)-C(6) \ -179.42(19) 
C(3)-C(4)-C(5)-N(9) \ 178.50(19) 
N(10)-N(9)-C(5)-C(4) \ -152.95(19) 
N(10)-N(9)-C(5)-C(6) \ 28.9(3) 
C(2)-C(1)-C(6)-C(5) \ 2.6(3) 
N(1)-C(1)-C(6)-C(5) \ -178.27(19) 
C(2)-C(1)-C(6)-N(12) \ -178.06(18) 
N(1)-C(1)-C(6)-N(12) \ 1.1(3) 
C(4)-C(5)-C(6)-C(1) \ 0.6(3) 
N(9)-C(5)-C(6)-C(1) \ 178.80(19) 
C(4)-C(5)-C(6)-N(12) \ -178.73(18) 
N(9)-C(5)-C(6)-N(12) \ -0.6(3) 
C(8)-N(12)-C(6)-C(1) \ 73.4(3) 
N(13)-N(12)-C(6)-C(1) \ -107.8(2) 
C(8)-N(12)-C(6)-C(5) \ -107.3(3) 
N(13)-N(12)-C(6)-C(5) \ 71.5(3) 
N(12)-N(13)-C(7)-N(14) \ 0.3(3) 
C(8)-N(14)-C(7)-N(13) \ -0.1(3) 
C(7)-N(14)-C(8)-N(12) \ -0.2(3) 
N(13)-N(12)-C(8)-N(14) \ 0.4(3) 
C(6)-N(12)-C(8)-N(14) \ 179.3(2) 

Symmetry transformations used to generate equivalent atoms:

Table S25. Hydrogen bonds for 7 [Å and °].

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Table S26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 8. U(eq) is defined as one third of the trace of the orthogonalized U^ij tensor.

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**Table S27.** Bond lengths [Å] and angles [°] for 8.
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N(8)-C(9) 1.328(4)
N(8)-N(9) 1.365(3)
N(8)-C(6) 1.422(3)
N(9)-C(10) 1.305(4)
N(10)-C(9) 1.298(4)
N(10)-C(10) 1.347(5)
C(1)-C(6) 1.365(4)
C(1)-C(2) 1.423(4)
C(2)-C(3) 1.413(4)
C(3)-C(4) 1.435(4)
C(4)-C(5) 1.416(4)
C(5)-C(6) 1.402(4)
C(7)-H(7) 0.9300
C(8)-H(8) 0.9300
C(9)-H(9) 0.9300
C(10)-H(10) 0.9300
C(7)-N(1)-N(2) 109.5(2)
C(7)-N(1)-C(1) 130.0(2)
N(2)-N(1)-C(1) 120.5(2)
C(8)-N(2)-N(1) 101.8(2)
C(7)-N(3)-C(8) 102.7(2)
C(2)-N(4)-H(4B) 115(2)
C(2)-N(4)-H(4A) 115(2)
H(4B)-N(4)-H(4A) 128(3)
O(2)-N(5)-O(1) 119.0(2)
O(2)-N(5)-C(3) 121.0(2)
O(1)-N(5)-C(3) 120.0(2)
C(4)-N(6)-H(6A) 120.0
C(4)-N(6)-H(6B) 120.0
H(6A)-N(6)-H(6B) 120.0
O(3)-N(7)-O(4) 122.8(3)
O(3)-N(7)-C(5) 119.4(3)
O(4)-N(7)-C(5) 117.7(3)
C(9)-N(8)-N(9) 110.1(2)
C(9)-N(8)-C(6) 129.7(3)
N(9)-N(8)-C(6) 120.2(2)
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Symmetry transformations used to generate equivalent atoms:

Table S28. Anisotropic displacement parameters (Å² x 10³) for 8. The anisotropic displacement factor exponent takes the form: -2π²[ h² a*² U₁₁ + ... + 2 h k a* b* U₁₂ ]

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Table S29. Hydrogen coordinates (Å x 10^4) and isotropic displacement parameters (Å^2 x 10^-3) for 8.

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Table S30. Torsion angles [°] for 8.

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Symmetry transformations used to generate equivalent atoms:

Table S31. Hydrogen bonds for 8 [Å and °].

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DSC plots for the title compounds

Fig. S5 DSC plot for compound 4

Fig. S6 DSC plot for compound 5
Fig. S7 DSC plot for compound 6

Fig. S8 DSC plot for compound 7
**Fig. S9** DSC plot for compound 8

**Fig. S10** DSC plot for compound 9
Theoretical study

All calculations were carried out at Gaussian 09 package. All molecules were optimized at DFT/B3LYP functional 6-31G** basis set, and the structures were conformed to be true local-energy minima on the potential-energy surface with frequency analysis. The change of enthalpy for the reactions at 298 K can be expressed as

\[ \Delta H_{298} = \sum \Delta_H^r - \sum \Delta_H^p \]  

(1)

where \( \Delta_H^r \) and \( \Delta_H^p \) are the HOF of reactants and products at 298 K, respectively, and \( \Delta H_{298} \) can be calculated using the following expression:

\[ \Delta H_{298} = \Delta E_{298} + \Delta ZPE + \Delta H_T + \Delta nRT \]  

(2)

where \( \Delta E_0 \) is the change in total energy between the products and the reactants at 0 K; \( \Delta ZPE \) is the difference between the zero-point energies (ZPE) of the products and the reactants at 0 K; \( \Delta H_T \) is thermal correction from 0 to 298 K. The \( \Delta(PV) \) value in eq (2) is the PV work term. It equals \( \Delta(nRT) \) for the reactions of ideal gas. For the isodesmic reactions, \( \Delta n = 0 \), so \( \Delta(PV) = 0 \). On the left side of Eq. (1), apart from target compound, all the others are called reference compounds. The HOF of reference compounds are available either from the experiments or from the high level computing like G2 method. Molar enthalpy of formation in solid state calculated by \( \Delta f H_s = \Delta f H_g - \Delta f H_{sub} \), enthalpy of formation in gas state (\( \Delta f H_g \)) was calculated by DFT method in combination with the isodesmic reactions, the sublimation enthalpy (\( \Delta f H_{sub} \)) was evaluated by the electrostatic potential method.

The detonation velocity and detonation pressure were calculated by the Kamlet-Jacobs formulas (3) and (4) as follows:

\[ D = 1.01(NM^{1/2}Q^{1/2})^{1/2} (1 + 1.30p) \]  

(3)

\[ P = 1.558p^2NM^{1/2}Q^{1/2} \]  

(4)

where \( D \) is the detonation velocity (km s\(^{-1}\)), \( P \) is the detonation pressure (GPa), \( N \) is the moles of detonation gases per gram of explosive, \( M \) is the average molecular weight (g mol\(^{-1}\)) of these gases. \( Q \) is the heat of detonation (cal g\(^{-1}\)), and is the loaded density (g cm\(^{-3}\)) of explosives.
Scheme 1 Isodesmic reaction

Table S32 Calculated total energy (E₀), zero point energy (ZPE), and thermal correction (Hₜ) and experimental gaseous heat of formation (ΔHₕgas) for the reference compounds. E₀ and ZPE are in (a.u.), Hₜ and HOF are in (kJ mol⁻¹).

<table>
<thead>
<tr>
<th>Compd.</th>
<th>ZPE</th>
<th>Hₜ</th>
<th>E₀</th>
<th>E_cor.</th>
<th>ΔHₜ</th>
<th>ΔHₕgas</th>
<th>ΔHₜ_sub</th>
<th>ΔHₕ_gas_solid</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄</td>
<td>0.04416</td>
<td>0.04692</td>
<td>-40.478950</td>
<td>-40.432030</td>
<td>10.01</td>
<td>-74.6ₚ</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NH₃</td>
<td>0.03377</td>
<td>0.03674</td>
<td>-56.523305</td>
<td>-56.486565</td>
<td>10.00</td>
<td>-45.9ₚ</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH₃CH₃</td>
<td>0.07303</td>
<td>0.07537</td>
<td>-79.759748</td>
<td>-79.684378</td>
<td>10.47</td>
<td>-84.0ₚ</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH₃NO₂</td>
<td>0.04894</td>
<td>0.05219</td>
<td>-244.963435</td>
<td>-244.911245</td>
<td>11.62</td>
<td>-74.7ₚ</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH₃N₃</td>
<td>0.04945</td>
<td>0.05364</td>
<td>-204.046787</td>
<td>-203.993147</td>
<td>14.22</td>
<td>238.4ₚ</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NH₂NH₂</td>
<td>0.05224</td>
<td>0.05522</td>
<td>-111.815351</td>
<td>-111.760131</td>
<td>11.06</td>
<td>93.4ₚ</td>
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<td></td>
</tr>
<tr>
<td>benzene</td>
<td>0.09861</td>
<td>0.10171</td>
<td>-232.157596</td>
<td>-232.055886</td>
<td>14.00</td>
<td>82.9ₚ</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,2,4-triazole</td>
<td>0.05877</td>
<td>0.06189</td>
<td>-242.195875</td>
<td>-242.133985</td>
<td>11.83</td>
<td>192.7ₚ</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.19248</td>
<td>0.20531</td>
<td>-1048.21335</td>
<td>-1048.00804</td>
<td>45.84</td>
<td>207.4₀</td>
<td>175.6ₚ</td>
<td>31.7ₚ</td>
</tr>
<tr>
<td>7</td>
<td>0.14956</td>
<td>0.16824</td>
<td>-1372.852635</td>
<td>-1372.684395</td>
<td>59.44</td>
<td>1253.6</td>
<td>239.0₁</td>
<td>1014.6₈</td>
</tr>
<tr>
<td>8</td>
<td>0.21441</td>
<td>0.22927</td>
<td>-1233.851790</td>
<td>-1233.622520</td>
<td>52.6₁</td>
<td>537.4₃</td>
<td>221.1₉</td>
<td>316.2₄</td>
</tr>
<tr>
<td>9</td>
<td>0.18548</td>
<td>0.20439</td>
<td>-1450.281089</td>
<td>-1450.076699</td>
<td>62.0₈</td>
<td>1239.2</td>
<td>264.6₆</td>
<td>974.6₂</td>
</tr>
</tbody>
</table>
The experimental data are taken from Ref. 4.

Table S33 Predicted heats of formation ($\Delta H_{\text{f,solid}}$), densities ($\rho$), detonation velocities ($D$), detonation pressures ($P$), and oxygen balance (OB) for the title compounds together with TNT, RDX and HMX

<table>
<thead>
<tr>
<th>Comp.</th>
<th>$\Delta H_{\text{f,solid}}$ (kJ mol$^{-1}$)</th>
<th>$\rho$ (g cm$^{-3}$)</th>
<th>$D$ (km s$^{-1}$)</th>
<th>$P$ (GPa)</th>
<th>OB (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>31.77</td>
<td>1.73</td>
<td>6.55</td>
<td>18.53</td>
<td>-91.36</td>
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<tr>
<td>7</td>
<td>1014.68</td>
<td>1.77</td>
<td>7.50</td>
<td>24.67</td>
<td>-58.07</td>
</tr>
<tr>
<td>8</td>
<td>316.24</td>
<td>1.73</td>
<td>6.56</td>
<td>18.67</td>
<td>-96.32</td>
</tr>
<tr>
<td>9</td>
<td>974.62</td>
<td>1.75</td>
<td>7.13</td>
<td>22.19</td>
<td>-74.95</td>
</tr>
<tr>
<td>TNT</td>
<td>-67.36</td>
<td>1.65</td>
<td>6.94</td>
<td>22.00</td>
<td>-73.97</td>
</tr>
</tbody>
</table>

References

[1] (a) G. M. Sheldrick, SHELXS-97, *Program for solution of crystal structures*, University of Gottingen, Germany, 1997; (b) G. M. Sheldrick, SHELXL-97, *Program for refinement of crystal structures*, University of Gottingen, Germany, 1997.


