

Supporting Information

Energetic polyazole polynitrobenzene and their coordination complexes

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Part A: Experimental section for polyazole polynitrobenzene **3a-f**, **4**, **6**, **7**.

General experimental methods.

Caution: For handling these energetic materials, small scale and best safety practices (leather gloves, face shield) are strongly encouraged to be used in undertaking preparation of polyazole polynitrobenzene (**3a-f**).

¹H, ¹³C NMR spectra were recorded on a 300 MHz Bruker Avance nuclear magnetic resonance spectrometer operating at 300.1, 282.4 and 75.5 MHz, respectively, using CDCl₃, CD₃CN and [D₆]DMSO as solvent unless otherwise indicated. Chemical shifts (¹H and ¹³C NMR) are reported relative to Me₄Si. The crystallization, melting and decomposition points were obtained on a differential scanning calorimeter at a scan rate of 10°C/min, respectively. Densities of solid salts were obtained at room temperature by employing a Micromeritics Accupyc 1330 gas pycnometer. Elemental analyses were determined using an Exeter CE-440 elemental analyzer.

General procedure for preparation polyazole polynitrobenzene **3a-f**.

To a round-bottomed flask fitted with a reflux condenser, is added 0.5 mmol 2-fluoro-1,3,5-trinitrobenzene (or 2,4-difluoro-1,3,5-trinitrobenzene, 1-amino-3,5-difluorotrinitrobenzen for diazole compound **3c-3d** and **3e**, or 1,3,5-trifluorotrinitrobenzene for triazole for tritriazole compound **3f**) in 15 mL benzene under nitrogen, and 0.5 mmol (1.0 mmol diazole compound **3c-3d**, **3e** or 1.5 mmol for triazole compound **3f**) 1-trimethylsilylimidazole or 1-trimethylsilyltriazole was added drop wise slowly. The yellow precipitate was yield immediately, then the reaction mixture was allowed to stir at room temperature overnight, the mixture was filtered, and washed with CH₂Cl₂ three times (3×5 mL) to give the crude product. The analytic pure sample was obtained by recrystalization from CH₃CN.

2-1H- imidazol-1-yl-1,3,5-trinitrobenzene (**3a**)¹: Yield 90%; yellow solid; IR (KBr): $\tilde{\nu}$ = 3107, 2361, 1610, 1549, 1345, 1078, 791, 650 cm⁻¹; Mp. (DSC) 216 °C (decomposition); ¹H NMR (CD₃CN): δ = 9.08 (s, 2H), 7.73 (s, 1H), 7.26 (s, 1H), 7.22 (s, 1H).

2-1H- triazol-1-yl-1,3,5-trinitrobenzene (**3b**)¹: Yield 90%; yellow solid; IR (KBr): $\tilde{\nu}$ = 3105, 2881, 1614, 1548, 1209, 1035, 918, 662 cm⁻¹; Mp. (DSC) 224 (melting point), 256 °C (decomposition); ¹H NMR (CD₃CN): δ = 9.08 (s, 2H), 8.67 (s, 1H), 8.20 (s, 1H).

The crude product was purified by silica gel column chromatography. The product was isolated using hexane-ethyl acetate (1:3) as eluent to give **3c**.

2,4-di-1H- imidazol-1-yl-1,3,5-trinitrobenzene (**3c**): Yield 60%; orange-yellow solid; IR (KBr): $\tilde{\nu}$ = 3151, 2967, 2823, 1613, 1541, 1307, 843, 708 cm⁻¹; Mp. (DSC) 156 °C (decomposition); ¹H NMR (CD₃CN): δ = 9.02 (s, 1H), 7.69 (s, 2H), 7.23 (s, 2H), 7.19 (s, 2H); C,H,N analysis (%): calcd for C₁₂H₇N₇O₆.H₂O (363.06): C 39.68, H 2.50, N 26.99; Found: C 40.34, H 2.30, N 26.43.

2,4-di-1H- triazol-1-yl-1,3,5-trinitrobenzene (**3d**): Yield 70%; yellow solid; IR (KBr): $\tilde{\nu}$ = 3130, 1602, 1550, 1508, 1337, 1129, 993, 868 cm^{-1} ; Mp. (DSC) 261 °C (decomposition); ^1H NMR (CD_3CN): δ = 9.09 (s, 1H), 8.67 (s, 2H), 8.22 (s, 2H); C,H,N analysis (%): calcd for $\text{C}_{10}\text{H}_5\text{N}_9\text{O}_6$ (347.04): C 34.59, H 1.45, N 36.31; Found: C 34.44, H 1.30, N 36.36.

1-Amino-3,5-di-1H-1,2,4-triazolyltrinitrobenzene (**3e**): Yield 80%; yellow solid; IR (KBr): $\tilde{\nu}$ = 3320, 1623, 1520, 1408, 1326, 1121, 933, 720 cm^{-1} ; Mp. (DSC) 298 °C (decomposition); ^1H NMR (CD_3CN): δ = 8.58 (s, 2H), 8.16 (s, 2H), 6.83 (s, 2H);
C,H,N analysis (%): calcd for $\text{C}_{10}\text{H}_6\text{N}_{10}\text{O}_6$ (362.05): C 33.16, H 1.67, N 38.07; Found: C 33.35, H 1.60, N 37.36.

2,4,6-tri-1H- triazol-1-yl-1,3,5-trinitrobenzene (**3f**): Yield 80%; yellow solid; IR (KBr): $\tilde{\nu}$ = 3115, 1773, 1558, 1508, 1335, 1276, 990, 665 cm^{-1} ; Mp. (DSC) 228 °C (decomposition); ^1H NMR (CD_3CN): δ = 8.71 (s, 3H), 8.25 (s, 3H); C,H,N analysis (%): calcd for $\text{C}_{12}\text{H}_6\text{N}_{12}\text{O}_6$ (414.05): C 34.79, H 1.46, N 40.57; Found: C 35.06, H 1.66, N 39.75.

Preparation of 2,3,4,6-tetra-1H- triazol-1-yl-1,3-dinitrobenzene (4): To a round-bottomed flask fitted with a reflux condenser, is added 0.5 mmol 2,4,6-trifluoro-1,3,5-trinitrobenzene in 15 mL benzene under dinitrogen, and 2.25 mmol 1-trimethylsilyltriazole was added drop wise slowly. The reaction mixture was allowed to stir at room temperature overnight, the mixture was filtered, and washed with CH_2Cl_2 three times (3×5 mL) to give the crude product. The crude product was purified by silica gel column chromatography. The first product was isolated using hexane-ethyl acetate (1:1) as eluent to give **3f** and the second product was isolated to give **4**.

2,4,6-tri-1H- triazol-1-yl-1,3,5-trinitrobenzene (**3f**): Yield 30%;

2,3,4,6-tetra-1H- triazol-1-yl-1,3-dinitrobenzene (**4**): Yield 50%; white solid; IR (KBr): $\tilde{\nu}$ = 3115, 1773, 1558, 1508, 1335, 1276, 990, 665 cm^{-1} ; Mp. (DSC) 228 °C (decomposition); ^1H NMR (CD_3CN): δ = 8.74 (s, 1H), 8.24 (s, 3H), 8.17 (s, 1H), 8.10 (s, 2H), 8.03 (s, 1H); C,H,N analysis (%): calcd for $\text{C}_{14}\text{H}_8\text{N}_{14}\text{O}_4$ (436.90): C 38.54, H 1.85, N 44.94; Found: C 38.38, H 1.71, N 44.60.

Preparation of 2,4,6-tri-1H- triazol-1-yl-3,5-dinitrophenol silver coordination complex, [Ag(TTDP)(H₂O)], **6, and 2,3,4,6-tetra-1H- tridazol-1-yl-1,3-dinitrobenzene silver dinitramide coordination complex, [Ag(TTDB)(CH₃CN)][N(NO₂)₂], **7**.** To a round-bottomed flask, is added 0.2 mmol 2,4,6-tri-1H- triazol-1-yl-1,3,5-trinitrobenzene, **3f**, or **4** and 0.2 mmol silver dinitramide in 30 mL acetonitrile-methanol (2:1). The solvent was slowly evaporated at room temperature after one week to give crystals.

[Ag(TTDP)(H₂O)] (**6**): Yield 35%; red crystal; IR (KBr): $\tilde{\nu}$ = 3435, 3126, 2361, 1614, 1552, 1392, 1130, 881 cm⁻¹; Mp. (DSC) 293 °C (decomposition); ¹H NMR (CD₃CN): δ = 8.96 (s, 2H), 8.53 (s, 1H), 7.99 (s, 1H), 7.97 (s, 2H); C,H,N analysis (%): calcd for C₁₂H₈AgN₁₁O₆ (436.09): C 28.25, H 1.58, N 30.20; Found: C 28.26, H 1.59, N 28.56.

[Ag(TTDB)(CH₃CN)][N(NO₂)₂] (**7**): Yield 55%; yellow crystal; IR (KBr): $\tilde{\nu}$ = 3430, 3126, 2270, 1562, 1519, 1277, 1187, 987 cm⁻¹; Mp. (DSC) 164 °C (decomposition); ¹H NMR (CD₃CN): δ = 7.56 (br, 8H); C,H,N analysis (%): calcd for C₁₆H₁₁AgN₁₈O₈ (690.01): C 27.80, H 1.60, N 36.47; Found: C 27.02, H 1.44, N 35.95.

Part B: DSC data for 3a-f, 4, 6, 7.

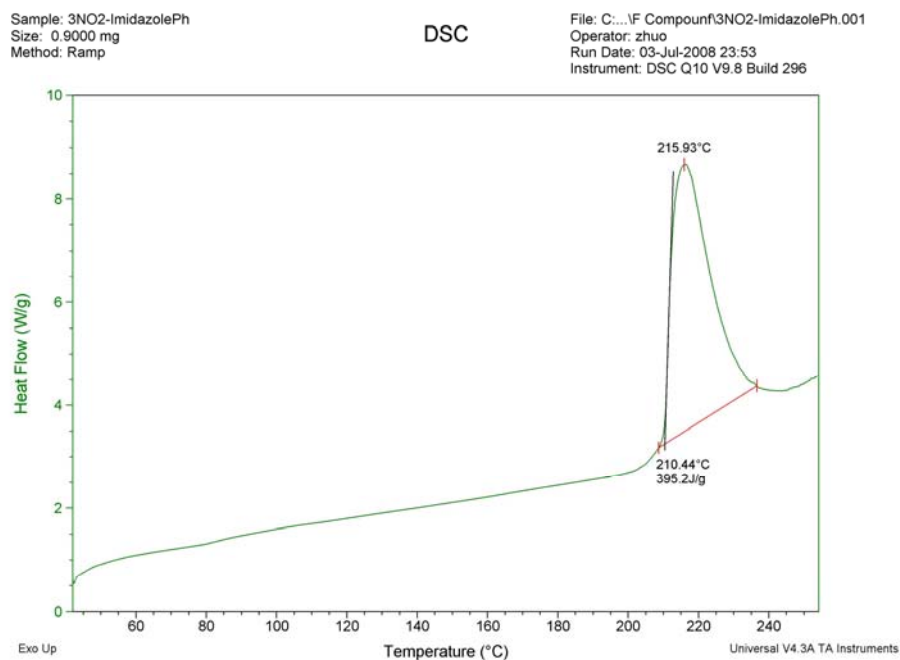


Figure B-1. Differential scanning calorimeter (DSC) figure for 2-1H- imidazol-1-yl-1,3,5-trinitrobenzene (3a).

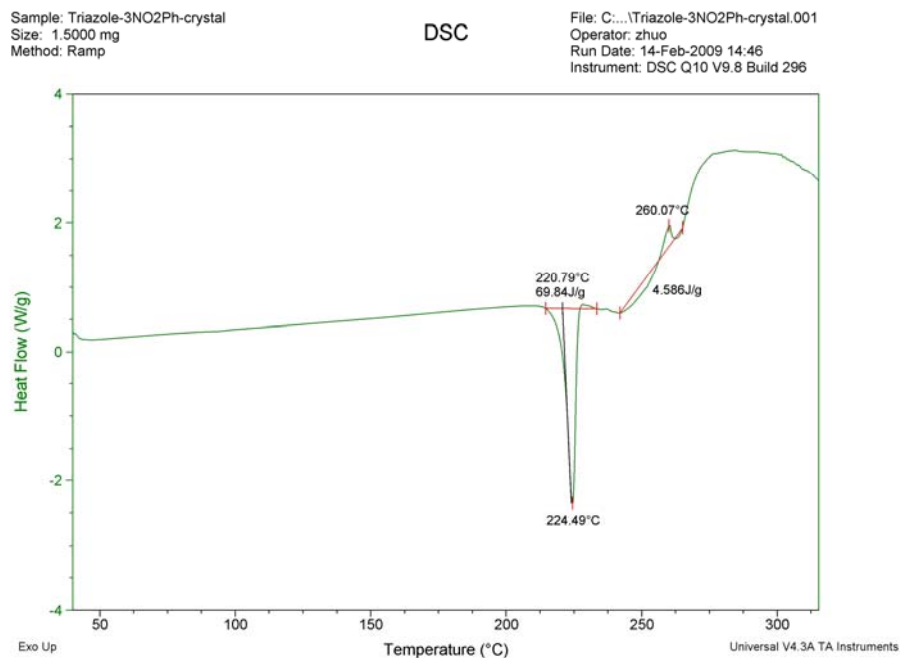


Figure B-2. Differential scanning calorimeter (DSC) figure for 2-1H- triazol-1-yl-1,3,5-trinitrobenzene (3b)

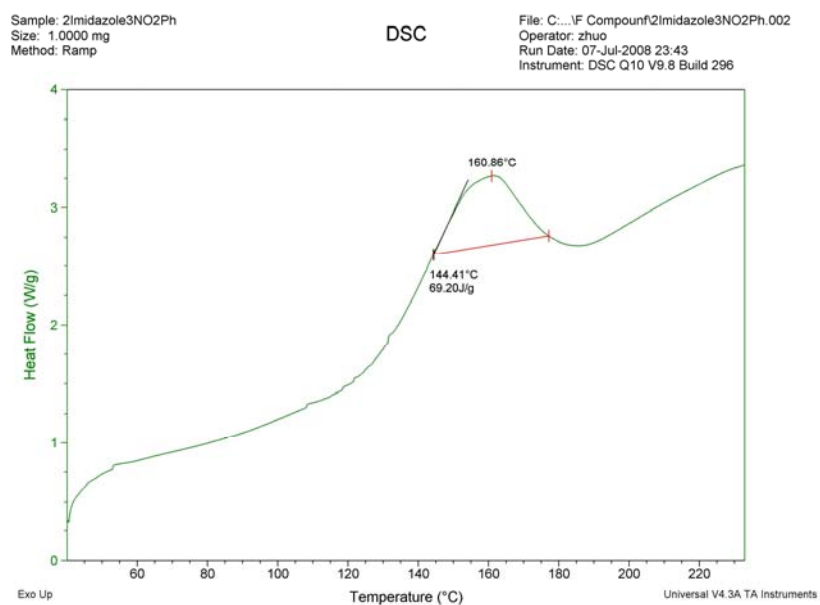


Figure B-3. Differential scanning calorimeter (DSC) figure for 2,4-di-1H- imidazol-1-yl-1,3,5-trinitrobenzene (3c)

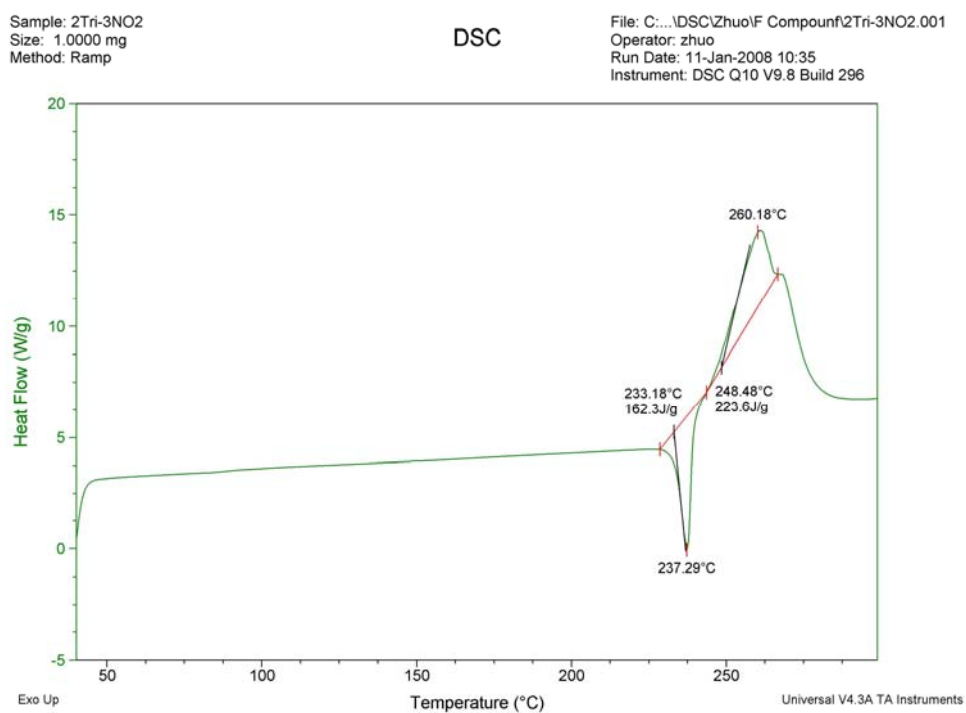
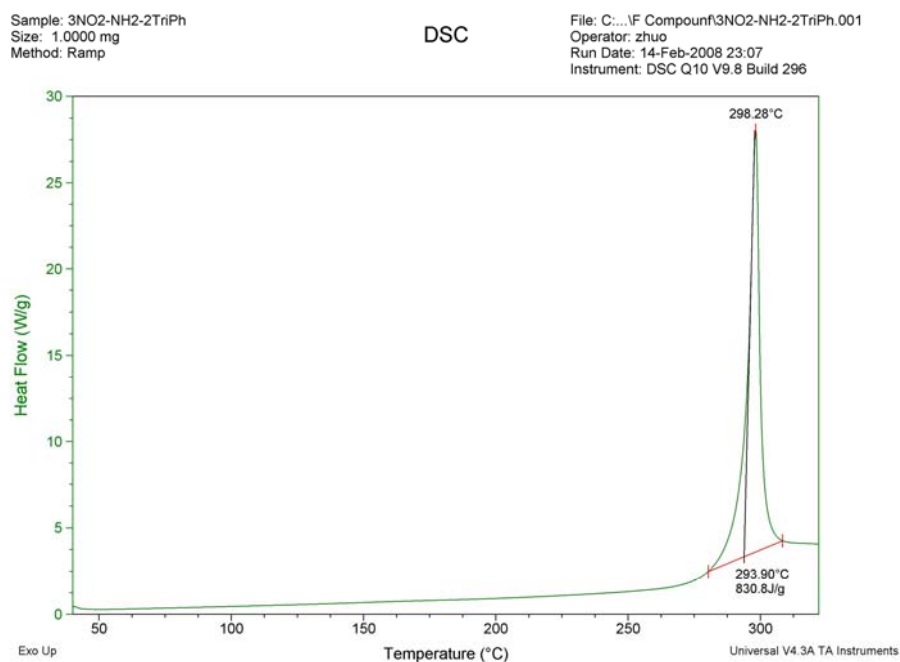
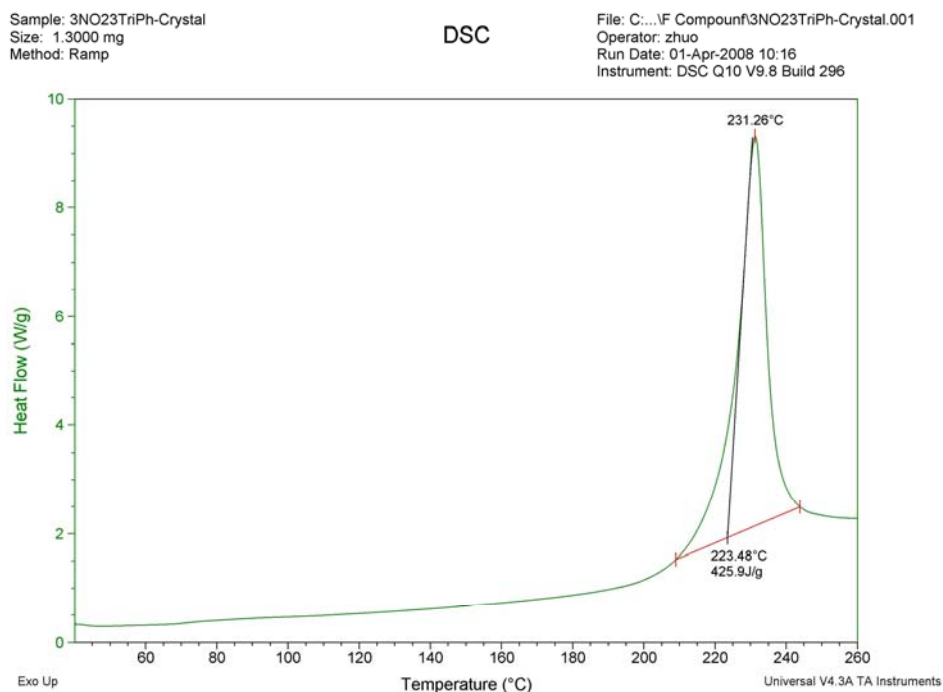


Figure B-4. Differential scanning calorimeter (DSC) figure for 2,4-di-1H- triazol-1-yl-1,3,5-trinitrobenzene (3d)



**Figure B-5. Differential scanning calorimeter (DSC) figure for
1-Amino-3,5-di-1H-1,2,4-triazolylnitrobenzene (3e)**



**Figure B-6. Differential scanning calorimeter (DSC) figure for 2,4,6-tri-1H- triazol-1-yl-1,3,5-trinitrobenzene
(3f)**

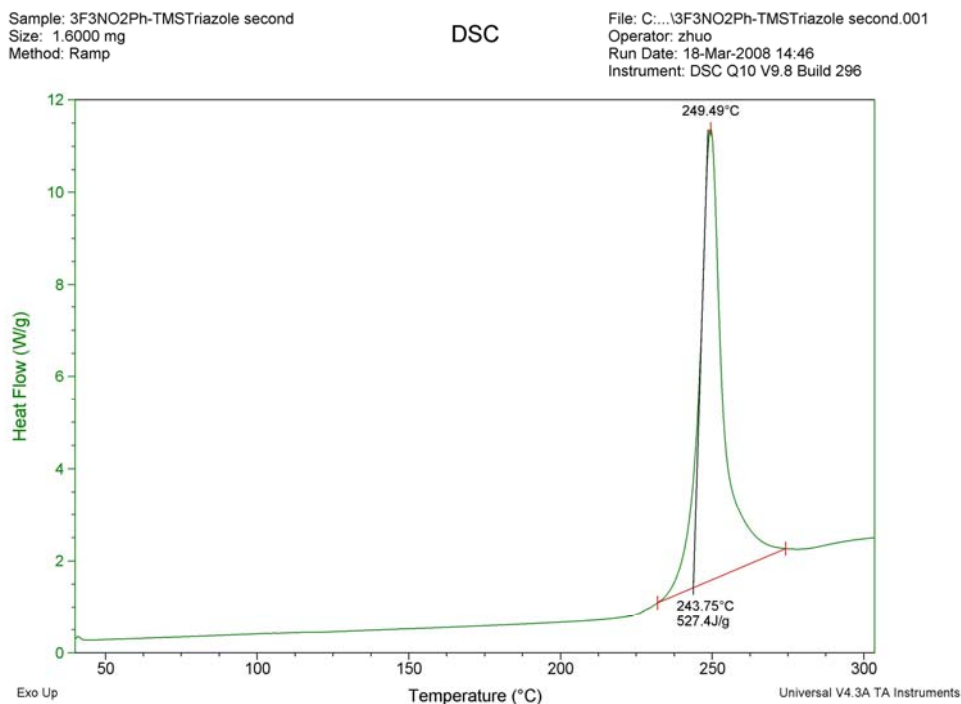


Figure B-7. Differential scanning calorimeter (DSC) figure for 2,3,4,6-tetra-1H- triazol-1-yl-1,3-dinitrobenzene (4)

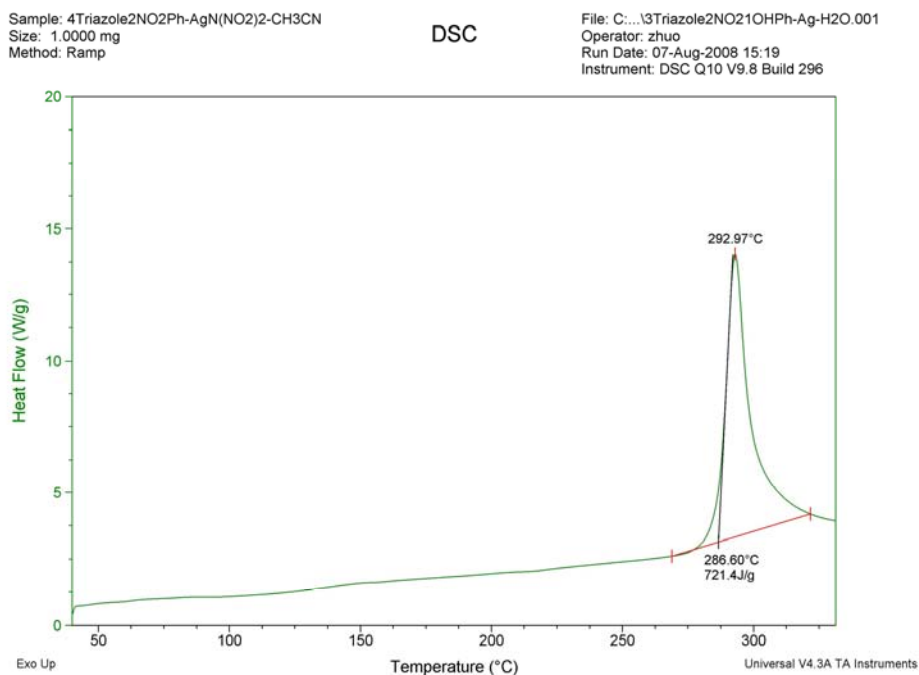


Figure B-8. Differential scanning calorimeter (DSC) figure for 2,4,6-tri-1H- triazol-1-yl-3,5-dinitrophenol silver coordination complex, [Ag(TTDP)(H₂O)] (6)

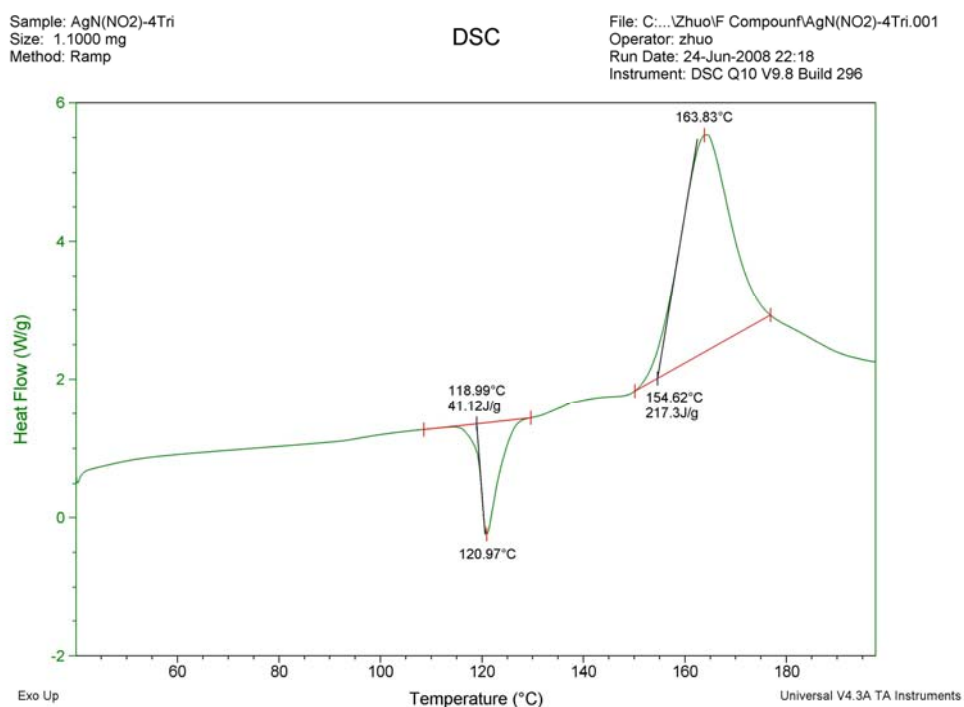


Figure B-9. Differential scanning calorimeter (DSC) figure for 2,3,4,6-tetra-1H-triazol-1-yl-1,3-dinitrobenzene silver dinitramide coordination complex, [Ag(TTDB)(CH₃CN)][N(NO₂)₂], 7

Part C: Crystallographic Data and Structure Refinement Parameters of compound 3e, 3f, 6, 7. CCDC 732611 (3e), 732612 (3f), 732613 (6), 732614 (7) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cifa

C-1. The Crystallographic Data and Refinement Parameters of compound 3e, 3f, 6, 7.

X-Ray Crystallography. Experimental

Crystals of compound **3e**, **3f**, **6** and **7** were removed from the flask, a suitable crystal was selected, attached to a glass fiber and data were collected at 90(2) K using a Bruker/Siemens SMART APEX instrument (Mo K α radiation, $\lambda = 0.71073$ Å) equipped with a Cryocool NeverIce low temperature device. Data were measured using omega scans 0.3° per frame for 5 seconds, and a full sphere of data was collected. A total of 2400 frames were collected with a final resolution of 0.77 Å for **3e** and 0.83 Å for **3f**, **6** and **7**. Cell parameters were retrieved using SMART² software and refined using SAINTPlus³ on all observed reflections. Data reduction and correction for Lp and decay were performed using the SAINTPlus software. Absorption corrections were applied using SADABS.⁴

Data for **3f** were rotationally twinned and were deconvoluted using CELL_NOW⁵ giving a two component twin relationship: 179.9° rotation about the reciprocal axis 1.000, 0.000, -0.001, with a refined twinning ratio of 0.3122(9). The matrix used to relate the second orientation to the first domain is: (1.000, 0.001, 0.037, 0.000, -1.000, 0.001, -0.003, -0.004, -1.000). Each cell component was refined using SAINTPlus on all observed reflections. Absorption corrections were applied using TWINABS.⁶

All structure were solved by direct methods and refined by least squares method on F² using the SHELXTL⁷ program package. Structures were solved in the space group P2(1)/c (# 14: **3e** and **3f**), C2/c (#15) and P-1 (#2: **7**) by analysis of systematic absences. Hydrogen atoms were added geometrically (riding model) unless stated below. All non-hydrogen atoms were refined anisotropically except in **7**; the solvent acetonitrile group was disordered in three positions, 41:39:20%, and these atoms were held isotropic with some geometrical restraints. In **6**, the solvent water molecules in the central voids were located but hydrogen atoms could not be located. They are included in the formula and weight. No decomposition was observed during data collection. Details of data collections and refinements are given in Table 1.

Table 1. Crystal Data and Structure Refinement Parameters for Compounds **3e-7**.

	3e	3f	6	7
Formula	C ₁₂ H ₉ N ₁₁ O ₆	C ₁₂ H ₆ N ₁₂ O ₆	C ₁₂ H ₁₂ AgN ₁₁ O ₈	C ₁₆ H ₁₁ AgN ₁₈ O ₈
CCDC no.	732611	732612	732613	732614
Fw	403.30	414.29	546.20	691.30
Crystal size (mm ³)	0.34x0.29x0.24	0.60x0.50x0.08	0.40x0.36x0.30	0.20 x 0.20 x 0.05
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	P2(1)/c	P2(1)/c	C2/c	P-1
a (Å)	9.6692(4)	12.2582(17)	20.041(3)	8.8611(4)
b (Å)	9.4624(4)	10.7107(15)	8.2412(8)	11.1986(5)
c (Å)	19.0356(8)	24.007(3)	24.046(3)	13.3871(6)
a (°)	-	-	-	78.4787(6)
b (°)	97.696(1)	92.253(2)	111.131(9)	74.2808(6)
g (°)	-	-	-	84.8365(7)
V (Å ³)	1725.95(13)	3149.5(7)	3704.4(8)	1252.07(10)
Z	4	8	8	2
D _c (g cm ⁻³)	1.552	1.747	1.959	1.834
μ (mm ⁻¹)	0.128	0.145	1.162	0.889
T (K)	90(2)	90(2)	90(2)	90(2)
λ _{MoKα} (Å)	0.71073	0.71073	0.71073	0.71073
Reflections collected	25293	72957	27473	18562
R(int)	0.0386	0.0423	0.0342	0.0354
Data/restraints/parameters	3967/0/263	7224/0/542	3333 / 0 / 290	5758/6/398
GOOF on F ²	1.083	1.055	1.082	1.071
R ₁ (I > 2σ(I)) ^a	0.0371	0.0382	0.0336	0.0341
wR ₂ (I > 2σ(I)) ^b	0.0932	0.0864	0.0863	0.0761
R (all data)	0.0436	0.0446	0.0372	0.0421
wR (all data)	0.0975	0.0909	0.0886	0.0802
Δρ _{min} and ρ _{max} (e/Å ³)	0.337 and -0.225	0.313 -0.273	and 0.954 -0.819	and 0.897 and -0.404

$$^a R = \sum ||F_o| - |F_c|| / \sum |F_o|. \quad ^b wR = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}.$$

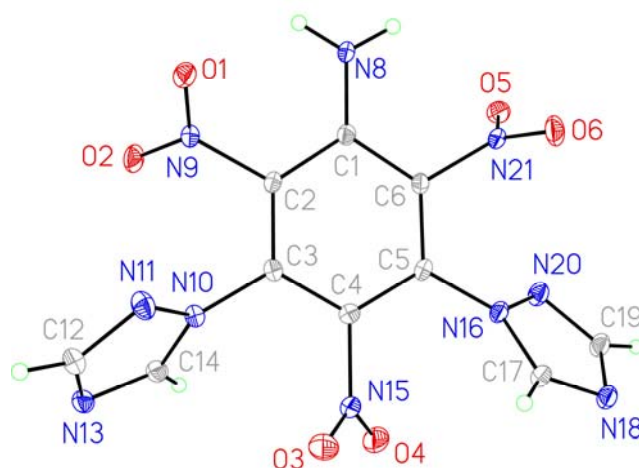


Figure C1-1. Structure of **3e** (displacement ellipsoids shown at 30% probability). Hydrogen atoms represented by spheres of arbitrary radius.

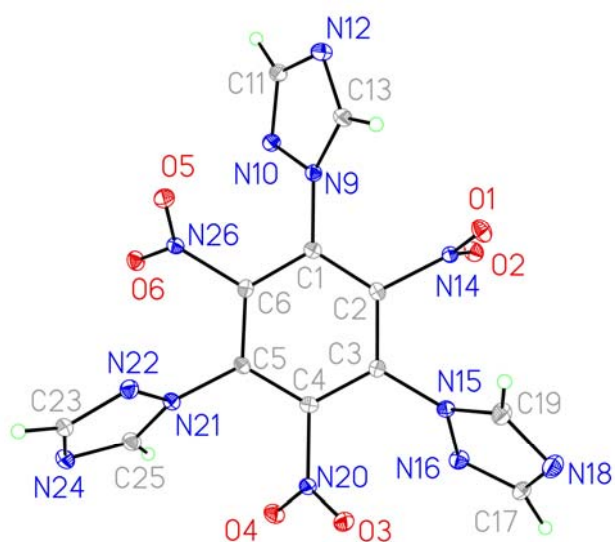


Figure C1-2. Structure of one of the unique molecule in the asymmetric unit of **3f** (displacement ellipsoids shown at 30% probability). Hydrogen atoms represented by spheres of arbitrary radius.

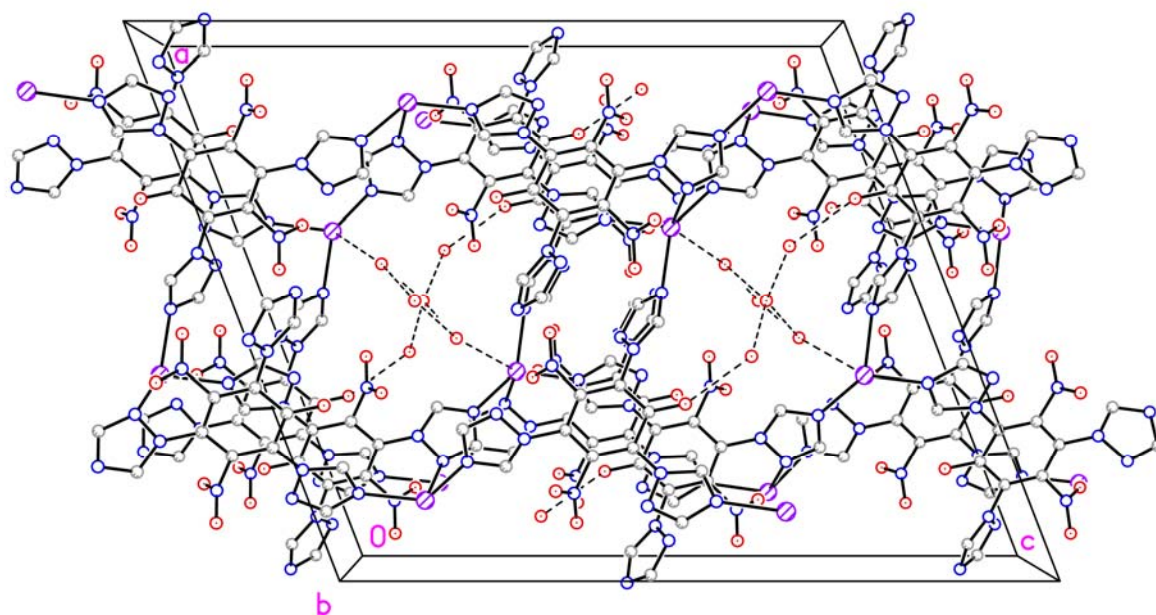


Figure C1-3. Packing diagram of **6** showing the honeycomb voids along the b-axis. Hydrogen atoms omitted for clarity. Dashed lines indicate close contacts.

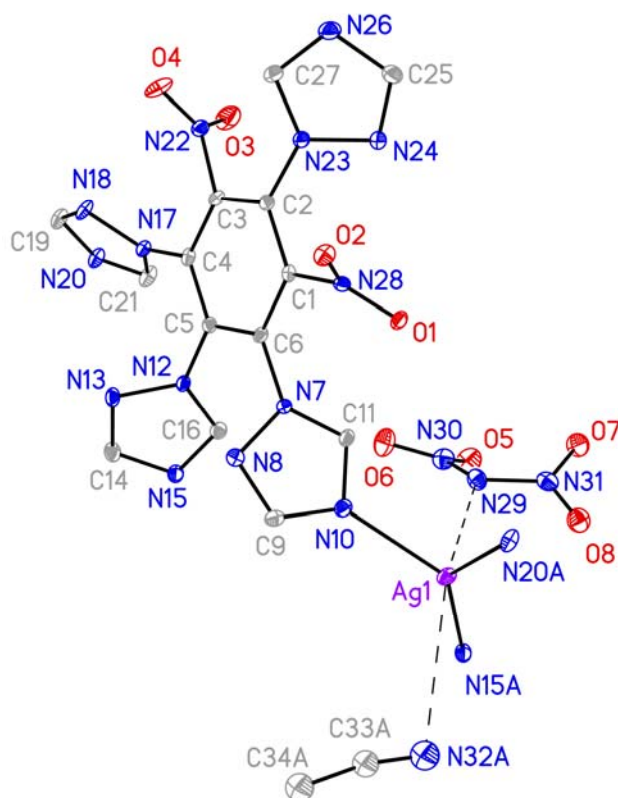


Figure C1-4. Structure of **7** (displacement ellipsoids shown at 30% probability). Hydrogen atoms omitted for clarity. Dashed lines indicate filled coordination sites by solvent (highest occupancy site shown) and dinitramide. Symmetry generated coordination atoms N15a and N20a also shown.

Structure Description:

The structure of the precursor molecules **3e** and **3f** are shown in Figures C2-1 and C2-2. Both crystallize in the monoclinic P2(1)/c system. **3e** has a solvent acetonitrile molecule co-crystallized in the lattice and in **3f** there are two crystallographically independent precursor molecules in the asymmetric unit. In **3e**, only the amino group is essentially coplanar to the ring system – all the other substituents form dihedrals ranging from 49.8° (N16-N20) to 72.3° (N21-O3) to the central ring. The amino group forms the basis of a rectangular hydrogen bonding synthon which binds **3e** into a corrugated sheet parallel to the ac plane. The solvent acetonitrile groups fill the void (void dimensions are ca. 8.9 x 9.6 Å) with a partial overlap of these voids across each corrugated sheet. The central ring in **3f** is fully nitrated, and in spite of close contacts, there are no classic H-bonding interactions. Due to the steric requirements of the nitrates and imidazoles there are a range of dihedral angles between each substituent and the central ring which gives rise to two crystallographically independent molecules in the asymmetric unit. Although not associated by hydrogen bonding, **3f** also packs in a corrugated fashion (parallel to the ac face also) albeit with a greater peak to peak amplitude. Extra figures and dihedral angle tables are given in the Supporting Information file. The reaction with AgN(NO₂)₂ to create dinitramide salts of **3f** and **4** led to the synthesis and isolation the unexpected product 2,4,6-tri-1H- triazol-1-yl-3,5-dinitrophenol silver monohydrate, [Ag(TTDP)(H₂O)], **6** and the desired 2,3,4,6-tetra-1H- triazol-1-yl-1,3-dinitrobenzene silver dinitramide coordination complex, [Ag(TTDB)(CH₃CN)][N(NO₂)₂], **7**. In **6** a complex honeycomb structure is formed with each Ag four coordinate (Ag1-N = 2.285 - 2.414). The phenolic O⁻ is stabilized by intra molecular H-bonding (C11-H11...O1 = 2.699(4)Å) and possibly by the solvent H₂O molecules. However the location of the hydrogen atoms associated with these water molecules presently cannot be determined. These solvent molecules lie in the honeycomb cavities which are oriented parallel to the b-axis as shown in Figure C2-4. However the more nitrogen containing, dinitramide complex **7** is shown in Figure C2-6. The silver atom is 5 coordinate and in a distorted trigonal bipyramid geometry in Figure C2-5. The weakly coordinated solvent acetonitrile was modeled in three major sites with Ag-N distances from 3.38, 2.765 and 2.599Å with occupancies of 41:20:39%. The imidazoles N10, N15 and N20 form the equatorial plane and the dinitramide, and disordered solvent MeCN molecule are the apical components of the coordination geometry (Ag-N = 2.339,

2.231, 2.324, 2.668 and 3.382Å respectively). The extended structure is in the form of an infinite 1D chain along the index (204). Although there are no classic hydrogen bonds there are very weak CH...O and CH...N interactions tying the whole structure into a 3D network.

C-2. Supporting Information for the Crystallographic Data and Refinement Parameters of compound 3e, 3f, 6, 7.

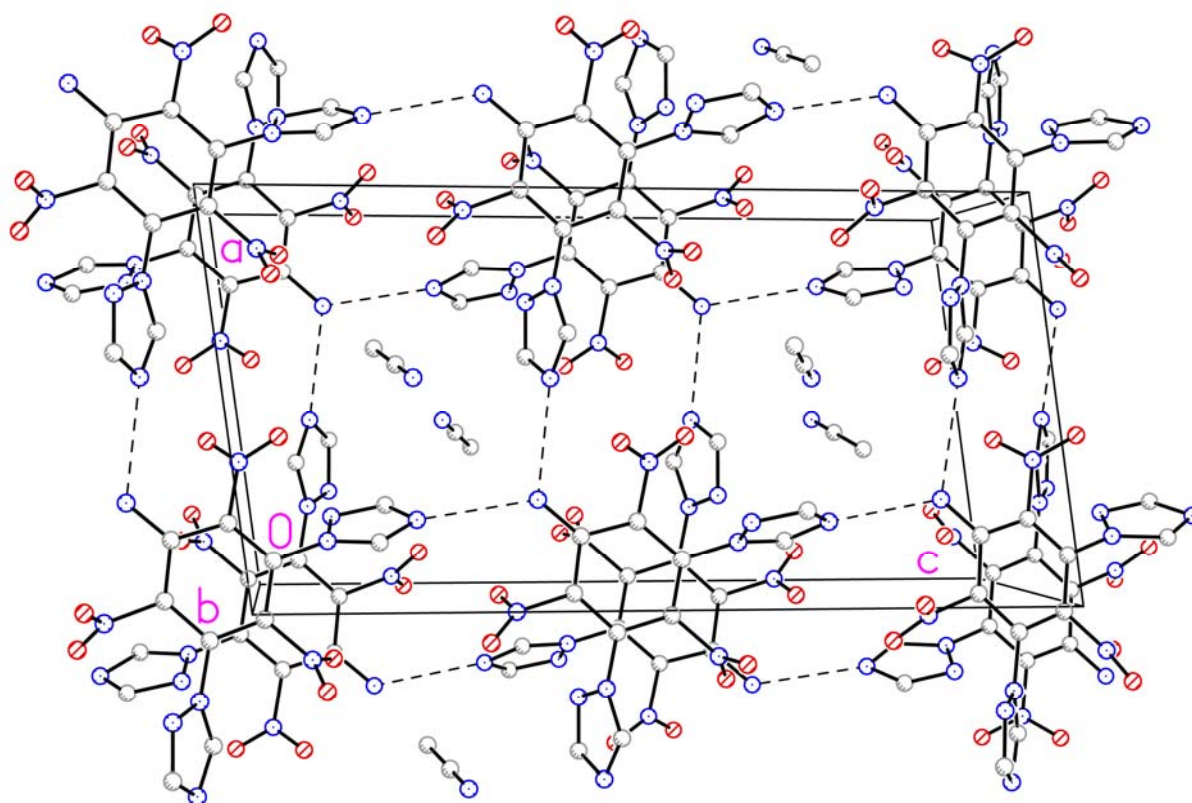


Figure C2-1. Packing Diagram of 3e showing the rectangular voids occupied by MeCN solvent molecules.

Table 2. Dihedral Angles of Substituents in 3e and 3f.

Cmpd	Substituent	Ring	Angle
3e	N9-O2	C1	55.8
3e	N10-C14	C1	62.5
3e	N15-O4	C1	56.4
3e	N16-N20	C1	49.8
3e	N21-O6	C1	72.3
3f	N9-C13	C1	54.9
3f	N4-O2	C1	84.5
3f	N15-O19	C1	62.9

3f	N20-O4	C1	62.9
3f	N21-C25	C1	68.6
3f	N26-O6	C1	58.1
3f	N32-C36	C26	61.2
3f	N37-O8	C26	94.6
3f	N38-C42	C26	53.1
3f	N43-O10	C26	61.1
3f	N44-C48	C26	86.1
3f	N49-O12	C26	55.2

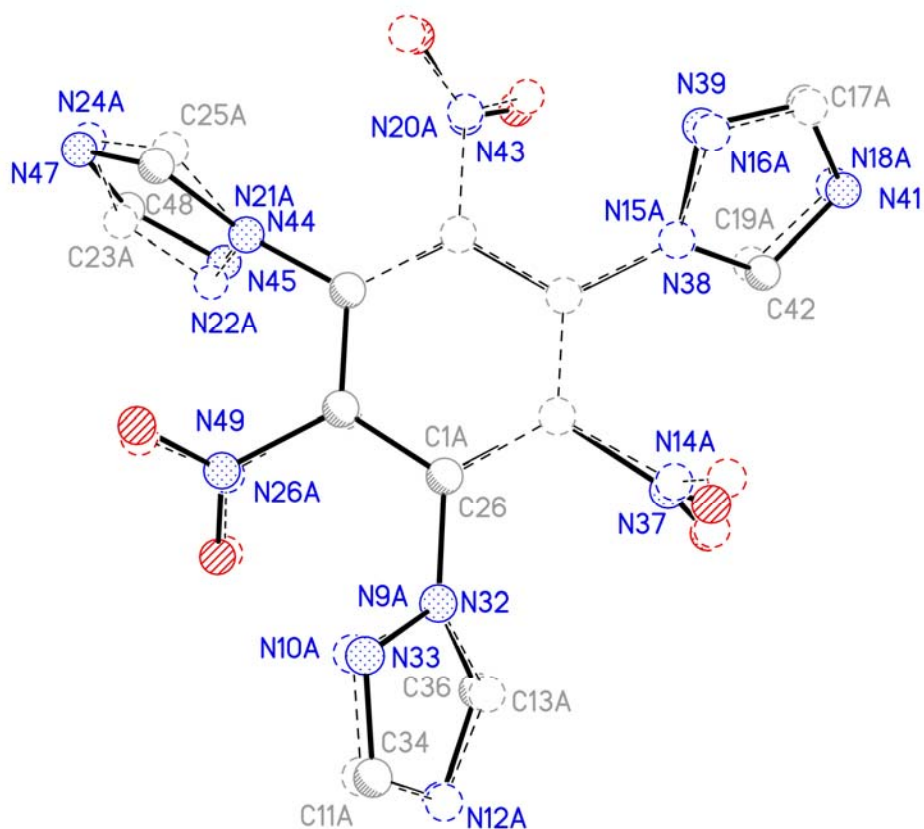


Figure C2-2. Overlay image of both independent molecules in 3f.

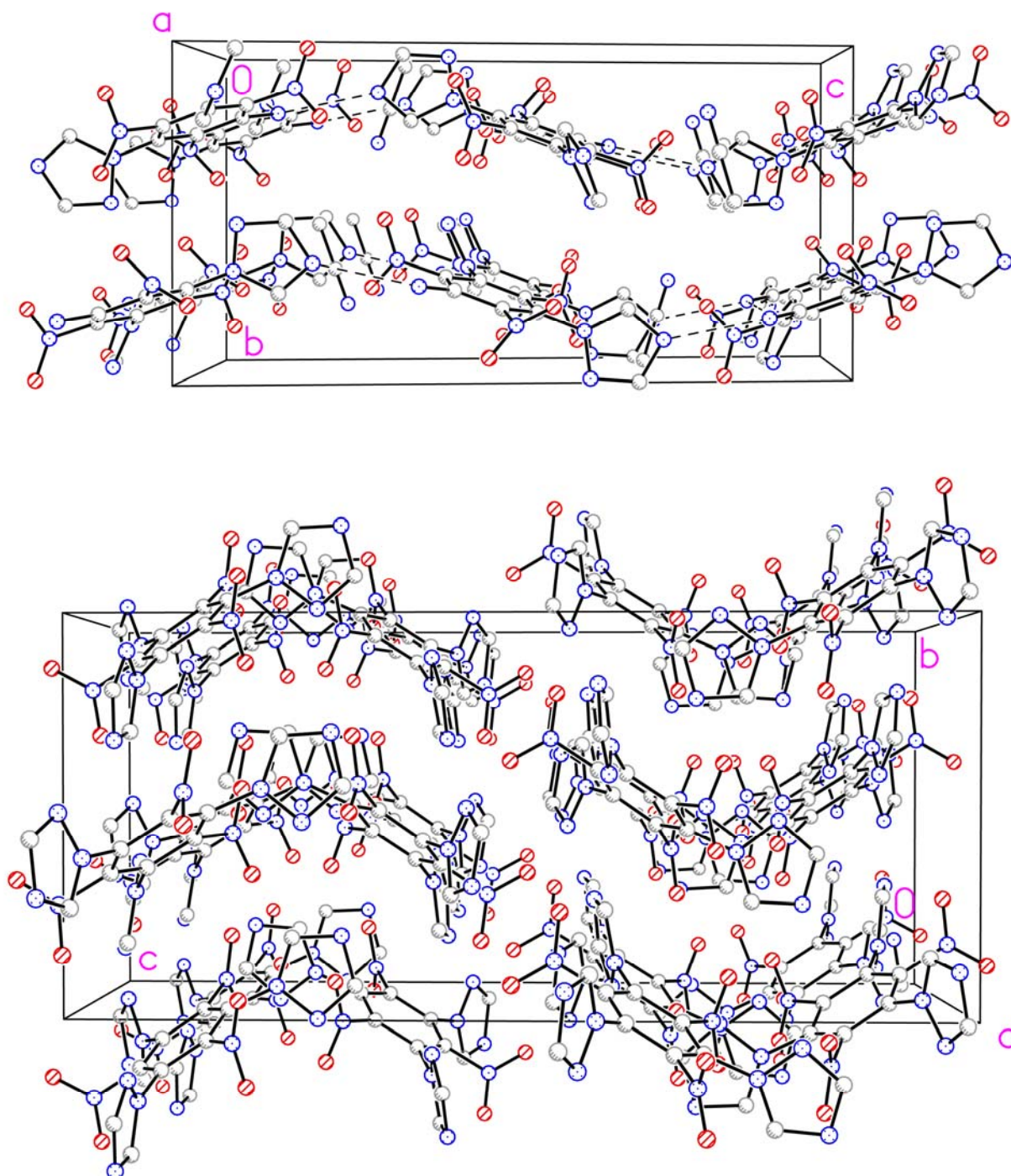


Figure C2-3. Packing diagrams of 3e (top) and 3f (bottom) showing the corrugated packing pattern.

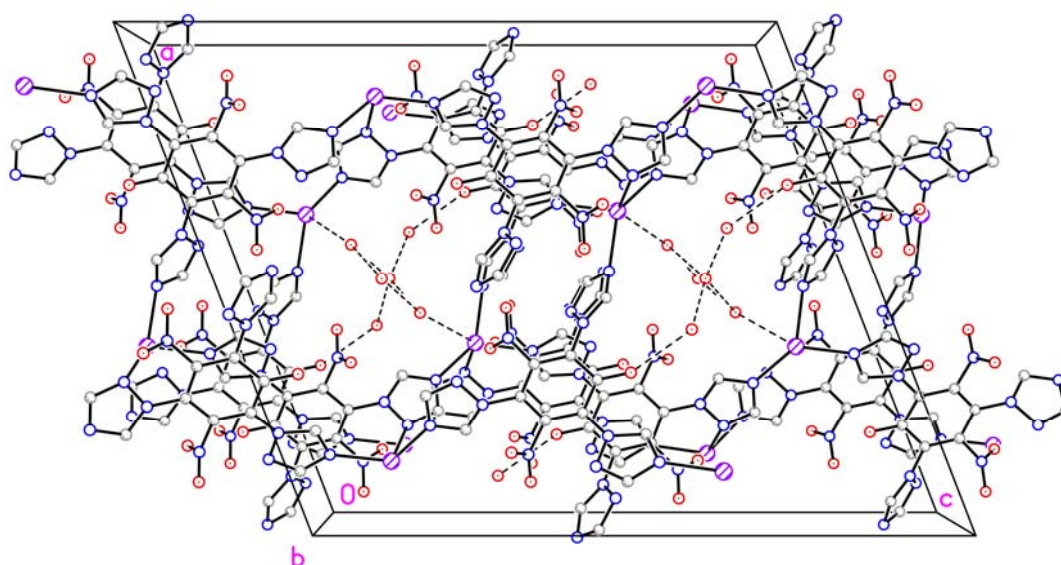


Figure C2-4. Packing diagram of **6** showing the honeycomb voids along the b-axis. Hydrogen atoms omitted for clarity. Dashed lines indicate close contacts.

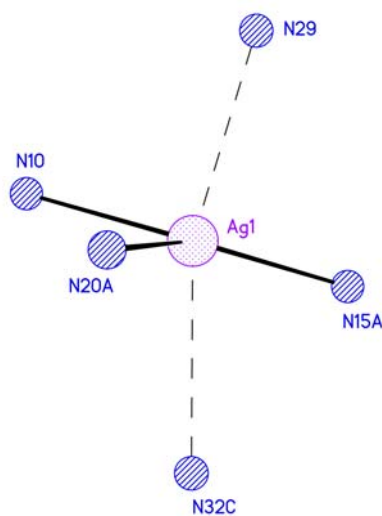


Figure C2-5. Distorted trigonal bipyramidal coordination of **7**. Angles are N10-Ag1-N15a = 130.2°; N15a-Ag1-N20a = 136.8°; N20a-Ag1-N10 = 92.2°; N29-Ag1-N32c = 161.8°.

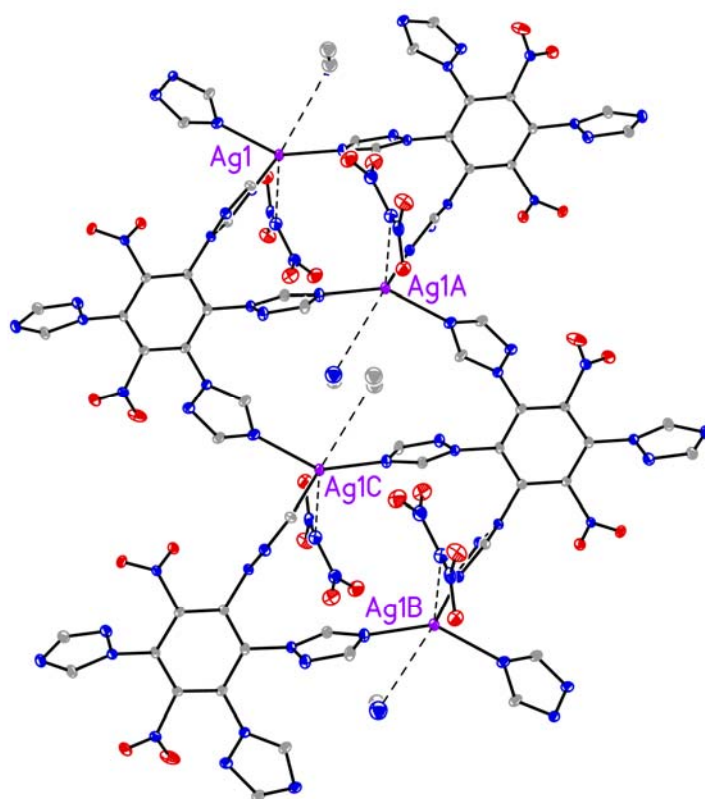
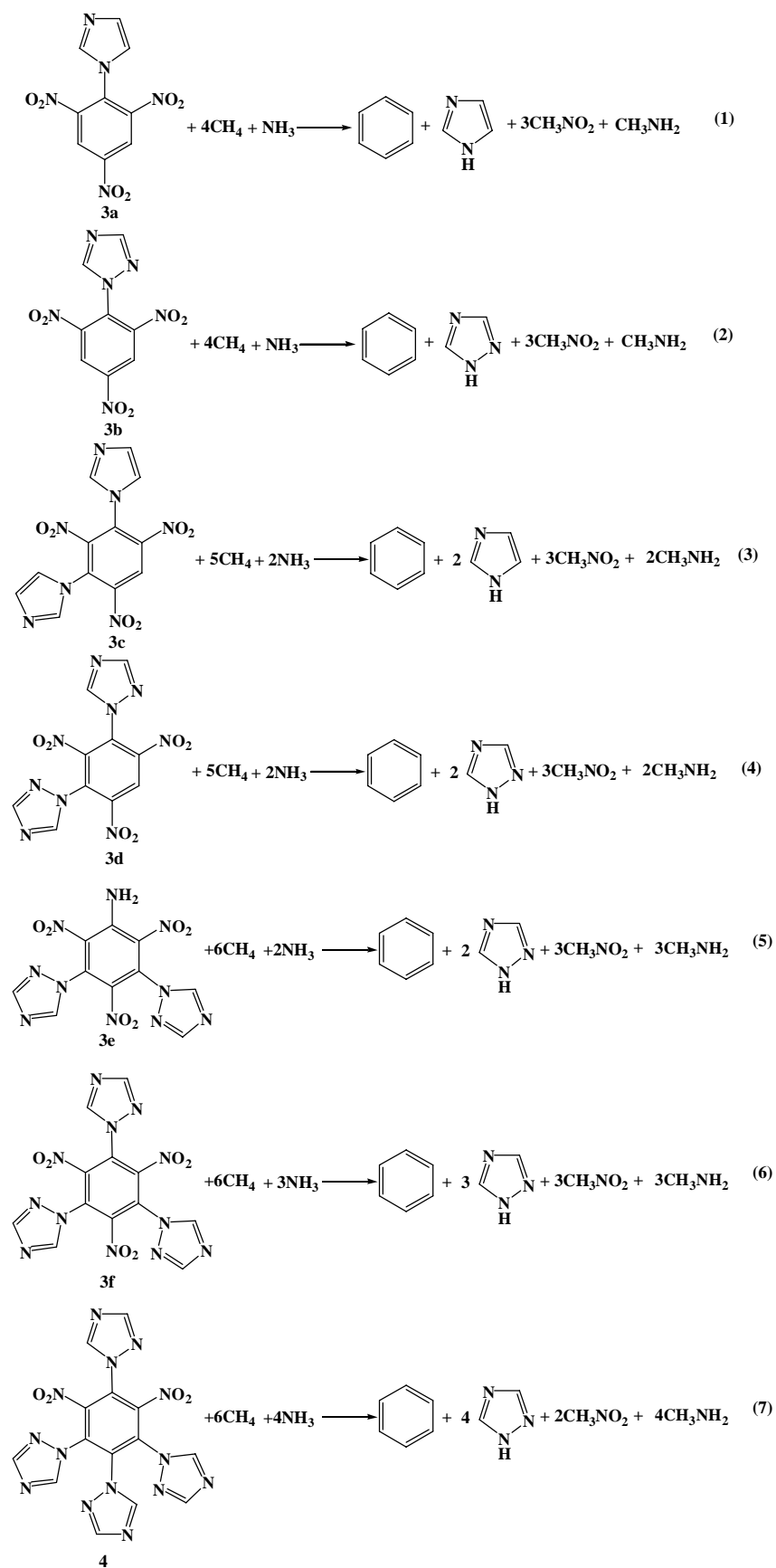


Figure C2-6. Section of the 1D chain in **7** (displacement ellipsoids shown at 30% probability) with the highest occupied solvent molecule position shown. Hydrogen atoms omitted and only silver atoms labeled for clarity.

Part D: *Ab Initio* computational data

Theoretical study.

Computations were performed by using the Gaussian03 (Revision D.01) suite of programs. The geometric optimization and the frequency analyses are carried out at the level of Becke three Lee-Yan-Parr (B3LYP) parameters up to 6-31+G(d,p) basis sets.⁸ All of the optimized structures were characterized to be true local energy minima on the potential energy surface without imaginary frequencies. The enthalpy of reaction ($\Delta H_{r,298}^{\circ}$) is obtained by combining the MP2/6-311++G** energy difference for the reaction, the scaled zero point energies, and other thermal factors. The heats of formation of the products were determined by using the method of isodesmic reactions (*Scheme 1*). The *Ab Initio* computational data are listed below



Scheme 1. Isodesmic reactions used for calculation of energetic materials.

TABLE 3. Calculated (B3LYP/6-31+G**//MP₂/6-311++G**) Total Energy (E_0), Zero-Point Energy (ZPE), Values of Thermal Correction (H_T), and Heats of Formation (HOF) of the polyazole polynitrobenzene compound.

Name	E_0 (au)	ZPE(au)	H_T (au)	HOF(kJ/mol)
3a	-1068.335478	0.157492	0.017204	167.6
3b	-1084.35972	0.146352	0.016823	361.8
3c	-1292.7848312	0.207794	0.021441	223.5
3d	-1324.8321837	0.185434	0.02069	476.4
3e	-1380.069408	0.202561	0.21831	651.82
3f	-1565.2985357	0.222691	0.023139	737.1
4	-1601.7038694	0.261998	0.025696	920.2
1,2,4-triazole	-241.6632438	0.059886	0.004507	190.3 ^[10]
CH ₄	-40.3796224	0.044793	10.0	-74.6 ^[10]
benzene	-231.5842377	0.100451	0.005346	82.9 ^[10]
NH ₃	-56.4154647	0.034384	0.003819	-45.9 ^[10]
CH ₃ NH ₂	-95.59384	0.06403	0.00438	-23 ^[10]
CH ₃ NO ₂	-118.76734	0.10328	0.005298	-103.8 ^[10]

Geometry Coordinates

B3LYP/6-31+G(d,p) optimized geometries (Å)

2-1H- imidazol-1-yl-1,3,5-trinitrobenzene (**3a**)

C	-0.49002000	0.07890500	-0.03709500
C	0.32524000	1.22733100	-0.01970600
C	1.71417700	1.16347600	-0.01459600
C	2.31530600	-0.08814700	-0.03824000
C	1.57167100	-1.26290100	-0.03767800

C	0.18795600	-1.15541500	-0.05274000
H	2.31221900	2.06548100	0.02641200
H	2.05889000	-2.23022600	-0.03400300
N	-0.26680200	2.57855900	0.03971900
O	-1.14240900	2.84439600	-0.77756300
O	0.18875100	3.34027700	0.88850400
N	-0.57221500	-2.42537800	-0.12255700
O	-1.41897500	-2.52092500	-1.00209400
O	-0.25813300	-3.29628200	0.68510600
N	3.79173400	-0.17418800	-0.04366200
O	4.28741300	-1.29801900	-0.03686800
O	4.41517100	0.88399100	-0.05505100
N	-1.89356400	0.13044000	0.07278000
C	-2.82247800	0.49085900	-0.89735600
H	-2.51958100	0.91222300	-1.84304000
C	-3.93763900	-0.30250200	0.75864400
H	-4.81311200	-0.58017200	1.32750300
N	-4.04260800	0.24492800	-0.50537200
C	-2.62766200	-0.40407800	1.13629800
H	-2.14808900	-0.76049900	2.03531000

2-1H- triazol-1-yl-1,3,5-trinitrobenzene (**3b**)

C	-0.24313900	-1.17382600	-0.06898600
C	0.42268300	0.05260000	-0.06762600
C	-0.33875600	1.22726800	-0.02290600
C	-1.73160400	1.17605700	-0.00969900
C	-2.34877400	-0.07181000	-0.01975200
C	-1.63024000	-1.26074500	-0.02908700
H	-2.31713100	2.08658500	0.01095800

H	-2.12780900	-2.22393400	0.00789300
N	0.31356600	2.56671600	-0.01094400
O	-0.27764300	3.47578800	0.54974800
O	1.40226300	2.66305400	-0.57393900
N	0.53586200	-2.43187600	-0.14364600
O	0.02470300	-3.41401200	0.37013600
O	1.62376500	-2.35339700	-0.70851900
N	-3.83757600	-0.13428200	-0.01933000
O	-4.34703900	-1.22289500	0.21254400
O	-4.42369000	0.92438200	-0.20631300
N	1.85606500	0.05611100	0.02522200
C	2.74858500	0.20797200	-0.94466900
H	2.54765600	0.40082100	-1.98827000
C	3.72958900	-0.15860200	0.98094700
H	4.51576200	-0.30574400	1.70833100
N	2.45081000	-0.20451600	1.23707300
N	3.94799400	0.06074200	-0.36735500
H	4.84553400	0.07516100	-0.84463300

2,4-di-1H- imidazol-1-yl-1,3,5-trinitrobenzene (**3c**)

C	-0.00000800	-0.54909600	-0.00000500
C	1.23962200	0.10799600	-0.00365700
C	1.19838400	1.51326100	0.00067100
C	-0.00001600	2.21351600	-0.00001000
C	-1.19841200	1.51325200	-0.00069000
C	-1.23964500	0.10798700	0.00364200
H	-0.00001900	3.29696200	-0.00001200
N	2.43294600	2.32091900	0.03126900
O	2.45789200	3.24899500	0.83593600

O	3.32007500	2.02422800	-0.76167900
N	0.00000600	-2.03331200	0.00000200
O	-0.31844000	-2.57934000	1.04874200
O	0.31853300	-2.57934100	-1.04871300
N	-2.43297600	2.32090800	-0.03130100
O	-3.32007400	2.02427400	0.76170300
O	-2.45790000	3.24900400	-0.83594500
N	2.43665800	-0.63550300	0.06371900
C	3.35423000	-0.87041400	-0.95389600
H	3.26676700	-0.39245600	-1.91741400
C	3.97975700	-2.05422100	0.72629400
H	4.60468000	-2.73283800	1.28843700
N	-2.43667500	-0.63551900	-0.06373100
C	-3.35427100	-0.87039300	0.95387500
H	-3.26684300	-0.39237800	1.91736800
C	-3.97972700	-2.05430800	-0.72626600
H	-4.60462400	-2.73296500	-1.28838900
N	4.27961200	-1.71006900	-0.57753800
N	-4.27962300	-1.71008900	0.57754000
C	2.84315300	-1.42127100	1.14759700
H	2.29871100	-1.42990400	2.07921100
C	-2.84312500	-1.42135900	-1.14757200
H	-2.29865100	-1.43004800	-2.07916700

2,4-di-1H- triazol-1-yl-1,3,5-trinitrobenzene (**3d**)

C	0.00003600	-0.54756700	-0.00003500
C	-1.23431200	0.12043400	0.02615400
C	-1.19824100	1.52535700	0.01941100
C	-0.00004900	2.22414100	-0.00003600

C	1.19819000	1.52543200	-0.01950000
C	1.23434100	0.12050200	-0.02625600
H	-0.00008400	3.30722700	-0.00001400
N	-2.42880200	2.33840000	0.00387400
O	-2.42614400	3.32344800	-0.72822700
O	-3.34666500	1.98826500	0.74060300
N	0.00009400	-2.03449200	0.00001400
O	0.56766500	-2.57995700	-0.93619400
O	-0.56730400	-2.57994000	0.93633900
N	2.42867800	2.33858800	-0.00388300
O	3.34658900	1.98862000	-0.74063100
O	2.42595200	3.32352300	0.72836800
N	-2.43011900	-0.62491200	-0.05744100
C	-3.42549300	-0.84942200	0.85771200
H	-3.48464300	-0.32924300	1.80063700
C	-3.72065400	-2.09212400	-0.81513500
H	-4.16638500	-2.81981600	-1.47825600
N	2.43016400	-0.62481200	0.05740100
C	3.42558700	-0.84933800	-0.85769600
H	3.48473800	-0.32925200	-1.80067000
C	3.72055100	-2.09215000	0.81511000
H	4.16619800	-2.81989800	1.47822800
N	-2.61230400	-1.45376300	-1.13991800
N	-4.25246400	-1.75924800	0.40075800
N	2.61239800	-1.45349900	1.13999500
N	4.25231100	-1.75944400	-0.40085100

1-Amino-3,5-di-1H-1,2,4-triazolyltrinitrobenzene (**3e**)

C	-1.16499000	-0.18363800	-0.02345400
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C	-1.26058600	1.21588300	-0.03864800
C	-0.11912700	2.06441600	0.00340200
C	1.14834300	1.40206600	0.01737300
C	1.26973400	0.00990800	0.01382800
C	0.10313400	-0.77125400	-0.00270100
N	2.35395900	2.23438000	0.04067900
O	2.39116400	3.20173500	-0.72837100
O	3.24097000	1.94000900	0.83417800
N	-2.57927200	1.83746800	-0.22412800
O	-3.34185800	1.33213500	-1.03705900
O	-2.81663300	2.86776500	0.41798600
N	0.22884700	-2.23591000	0.11491300
O	0.82611900	-2.66220700	1.09829100
O	-0.28615500	-2.91540000	-0.76719800
N	-0.21524600	3.40843200	0.02071700
H	0.57982400	3.96907700	-0.24958300
H	-1.11984800	3.83383100	0.16937700
N	-2.34034300	-0.95879800	0.09511200
C	-2.93541200	-1.84292100	-0.76708200
H	-2.46136700	-2.18661500	-1.67282300
C	-4.23217000	-1.45974000	0.84522600
H	-5.09618800	-1.51030500	1.49248000
N	2.52110100	-0.64851400	-0.05467800
C	3.50031000	-0.84495900	0.88315500
C	3.91243600	-2.02227000	-0.81121200
H	3.50110800	-0.35346600	1.84289200
H	4.41657200	-2.70530500	-1.48004300
N	2.77855400	-1.43821900	-1.15137500
N	4.39146800	-1.69313500	0.42692200
N	-3.19983500	-0.69166300	1.13520300

N	-4.11908800	-2.18039300	-0.31254100
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2,4,6-tri-1H- triazol-1-yl-1,3,5-trinitrobenzene (**3f**)

C	0.18467000	1.40081300	-0.00324500
C	-1.09397100	0.83958200	-0.00981200
C	-1.30612900	-0.54058200	-0.00320200
C	-0.18071200	-1.36724600	-0.01050400
C	1.12067700	-0.86090200	-0.00352400
C	1.27400200	0.52710500	-0.01021400
N	-0.37451800	-2.83547200	0.03230500
O	-0.43657700	-3.32540100	1.15730100
O	-0.45284400	-3.41731300	-1.03547400
N	-2.26850000	1.74171000	0.03222800
O	-2.66033800	2.04344100	1.15691800
O	-2.73293100	2.09979600	-1.03591500
N	2.64247500	1.09327600	0.03310600
O	3.18524200	1.31794300	-1.03442800
O	3.09857300	1.28098100	1.15836900
N	-2.61468600	-1.08179800	0.00660000
C	-3.42169000	-1.40596200	1.06466200
H	-3.12248200	-1.27421400	2.09508200
C	-4.41987900	-1.83361600	-0.73790200
H	-5.18858300	-2.15661900	-1.42529600
N	0.36955800	2.80476200	0.00680100
C	0.47294400	3.66824100	1.06493500
H	0.41969800	3.34569600	2.09536700
C	0.63483300	4.74225400	-0.73750600
H	0.75161500	5.56789800	-1.42483500
N	2.24380100	-1.72336800	0.00797500

C	2.93111000	-2.25372700	1.06728300
H	2.66902400	-2.05608200	2.09728900
C	3.79706000	-2.91296900	-0.73385200
H	4.46013700	-3.42002300	-1.42012900
N	-3.26541700	-1.36041400	-1.17112200
N	-4.56267200	-1.88061700	0.62261300
N	0.47524800	3.50485800	-1.17080500
N	0.64004500	4.89269700	0.62299100
N	2.80821100	-2.15311000	-1.16880800
N	3.91275400	-3.00540400	0.62692500

2,3,4,6-tetra-1H- triazol-1-yl-1,3-dinitrobenzene (**4**)

C	1.70293800	0.06848200	-0.03149700
C	0.94259700	1.23976300	0.00503600
C	-0.45893900	1.21735300	0.03359300
C	-1.12181200	-0.02350600	0.03576900
C	-0.37688100	-1.22054200	0.04377200
C	1.01823100	-1.15360800	0.00409700
N	1.79787300	-2.40773900	-0.08327900
O	2.46673200	-2.56208500	-1.09746300
O	1.69576800	-3.19170100	0.85275800
N	1.64869900	2.53470500	0.14240200
O	2.34769700	2.89128100	-0.79641100
O	1.49412600	3.12012800	1.20708000
N	3.11495200	0.08656100	-0.00849300
C	4.02342900	0.50689600	-0.94506100
C	5.03574900	-0.45775100	0.62824300
H	3.73839400	1.02783300	-1.84629000
H	5.84031100	-0.85563500	1.23014500

N	-1.17474200	2.42798800	0.07256000
C	-2.17979700	2.83768900	0.90448500
C	-1.70773100	4.38832500	-0.43379700
H	-2.59098100	2.21817600	1.68815900
H	-1.73388000	5.34379000	-0.93767900
N	-2.53441700	-0.06830000	0.00402800
C	-3.41435800	-0.65589100	0.86924300
C	-4.48073700	0.25617100	-0.69518000
H	-3.10583200	-1.18942300	1.75724000
H	-5.30484900	0.58641000	-1.31118400
N	-1.05138600	-2.46596600	-0.01652000
C	-1.19542100	-3.44832600	0.92657000
C	-2.34103300	-3.93502600	-0.76977800
H	-0.68602000	-3.42787300	1.87852900
H	-2.99595500	-4.47777300	-1.43638300
N	3.77614400	-0.56070700	1.00856000
N	5.23687300	0.18537300	-0.56244900
N	-1.80756900	-2.77843700	-1.11933400
N	-2.00078100	-4.38376500	0.47723300
N	-0.86371700	3.44110200	-0.79560900
N	-2.53360500	4.06660200	0.60980500
N	-3.22862700	0.52677300	-1.01591500
N	-4.64729400	-0.46228400	0.45798100

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