Supporting Information

Synthesis and characterization of the potential polycyclic energetic materials: using bicyclic triazole and azetidine structures as building blocks

Xin-bo YANG[a,b,#], Chen-hui JIA[c,#], Xiang-yan MIAO[a], Yu-chuan LI[a,*], Si-ping PANG[a,*]

[a] *School of Materials Science & Engineering, Beijing Institute of Technology, Beijing 100081, China.*

[b] *School of Mechatronical Engineering, Beijing Institute of Technology, Beijing 100081, China.*

[c] *Beijing Composite Materials Co., Ltd, No.261 Kangxi Road, Badaling Economic Development Zone, Yanqing District, Beijing, 102101, China.*

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1. Single Crystal X-ray Crystallography

Single crystal X-ray diffraction data for TCBT, compound **1**, **2** and **3** were collected using a Rigaku AFC10K Saturn. Single crystal of suitable quality was chosen and purged with a cooled nitrogen gas stream at different temperatures throughout the data collection. Data were collected and processed using Olex2[1] software. Structure was solved by direct methods and SHELX[2] was used for structure solution and least-squares refinement. The non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined using the riding model.

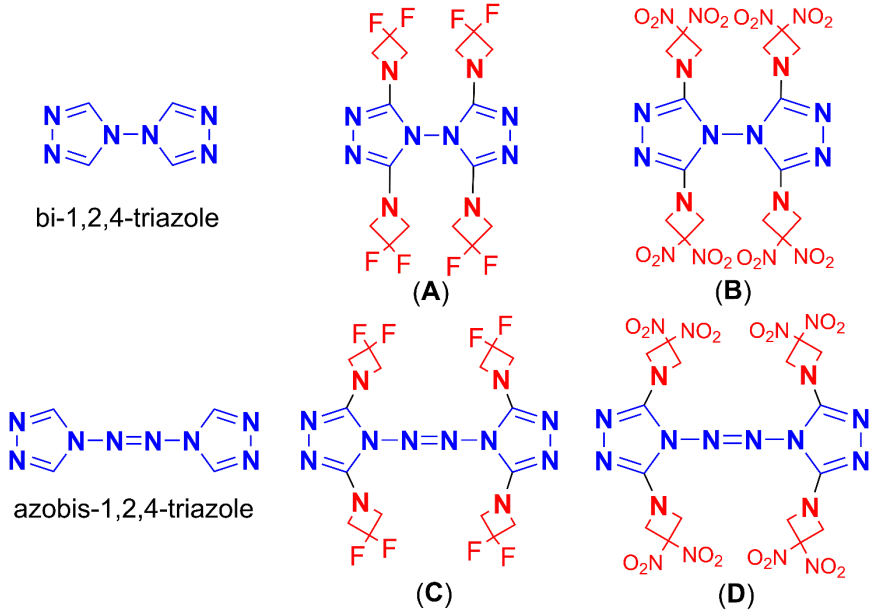
Table S1 Single Crystal X-ray Crystallography data for compounds

Compound	**TCBT**	**1**	**2**	**3**
CCDC No.	-	1589971	1589973	1589972
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Empirical formula	$C_4Cl_4N_6$	$C_{10}H_8Cl_2F_4N_{10}$	$C_{10}H_8Cl_2F_4N_8$	$C_9H_{10}Cl_2F_2N_8$
Formula weight	273.90	415.16	387.14	339.15
Temperature/K	113	153.15	296(2)	296(2)
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic
Space group	*C*2/c	$P2_1/c$	*P*-1	*P*-1
Unit cell dimensions	a=11.580(4) Å *α*=90° b=7.643(3) Å *β*=105.306(6)° c=11.117(4) Å *γ*=90°	a=10.950(2) Å *α*=90° b=7.2595(15) Å *β*=97.03(3)° c=9.6370(19) Å *γ*=90°	a=7.8331(10) Å *α*=100.654(10)° b=8.6308(10) Å *β*=94.011(10)° c=11.2924(10) Å *γ*=94.851(10)°	a=7.6743(13) Å *α*=92.753(4)° b=8.1690(14) Å *β*=93.733(4)° c=11.2815(19) Å *γ*=93.499(4)°
Volume/Å^3	949.0(6)	760.3(3)	744.724(15)	703.5(2)
Z	4	2	2	2
Density/g·cm^3	1.917	1.813	1.726	1.601
Crystal size/mm^3	0.18×0.16×0.14	0.23×0.21×0.1	0.220×0.200×0.180	0.220×0.200×0.180
θ(max)/°	3.23-27.515	3.375-27.487	1.842-24.906	2.501-25.058
μ/mm^{-1}	1.212	0.494	0.494	0.491
F(000)	536.0	416.0	388.0	344.0
Goodness-of-fit on F^2	1.129	1.133	0.996	0.972
Index ranges	-14 ≤ h ≤ 14, -9 ≤ k ≤ 9, -14 ≤ l ≤ 14	-14 ≤ h ≤ 14, -9 ≤ k ≤ 9, -12 ≤ l ≤ 12	-9≤h≤9, -10≤k≤10, 0≤l≤13	-9≤h≤6, -9≤k≤9, -13≤l≤13
R_1/wR_2 [I>2σ(I)]	0.0199/0.0535	0.0469/0.1049	0.0508/0.1611	0.0419/0.1196
R_1/wR_2 (all data)	0.0207/0.0539	0.0491/0.1062	0.0671/0.1784	0.0571/0.1343

2. Effect of the structure of azetidine on the density of the system.

In order to explore the influence of the structure of azetidine on the density of bicyclic triazole, we hypothesized four molecules: 3,3',5,5'-tetra(3,3-difluoroazetidine)-4,4'-bi-1,2,4-triazole (**A**), 3,3',5,5'-tetra(3,3-dinitroazetidine)-4,4'-bi-1,2,4-triazole (**B**), 3,3',5,5'-tetra(3,3-difluoroazetidine)-4,4'-azobis-1,2,4-triazole (**C**), 3,3',5,5'-tetra(3,3-dinitroazetidine)-4,4'-azobis-1,2,4-triazole (**D**). By calculating the density[3] of these four ideal molecules and comparing with the density of azobis-1,2,4-triazole and bi-1,2,4-triazole, we can fully explain the influence of the structure of azetidine on the density of the system.

From **Table S2**, the results show that the introduction of azetidine structure into the triazole system can indeed improve the molecular density.



Scheme S1 The designed triazolyl polycyclic compound **A**, **B**, **C** and **D**.

Table S2 Calculated density (g/cm^3) of triazolyl polycyclic compound and bi-1,2,4-triazole/azobis-1,2,4-triazole.

Compounds	α	β	γ	Molecular density	$v\sigma_{tot}^2$	Crystal density
bi-1,2,4-triazole	0.9183	0.0028	0.0443	1.485	58.47295	1.572
azobis-1,2,4-triazole	0.9183	0.0028	0.0443	1.532	47.54333	1.584
A	0.9183	0.0028	0.0443	1.763	36.42043	1.766
B	0.9183	0.0028	0.0443	1.823	23.62477	1.784
C	0.9183	0.0028	0.0443	1.780	30.25527	1.763
D	0.9183	0.0028	0.0443	1.819	23.63411	1.781

3. Infrared spectrum, mass spectrum, nuclear magnetic resonance spectrum of synthesized substances.

The FTIR spectra were obtained from KBr pellets using a Nicolet Magna FTIR 560 spectrophotometer (Madison, WI, USA) over the range of 400–4000 cm^{-1}. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on a Bruker ARX-400 instrument (Zurich, Switzerland). Chemical shifts are reported in ppm relative to tetramethylsilane. Liquid chromatography (LC)-MS electrospray ionization (ESI) data were acquired with an Agilent 6120 LC-MS spectrometer (Santa Clara, CA, USA).

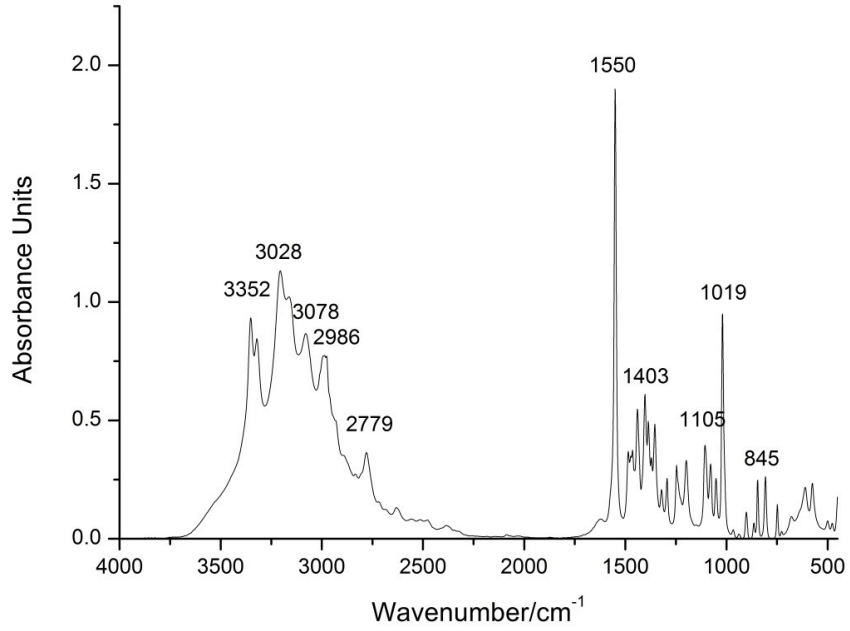


Figure S1. The FTIR spectrum of 1-tertiary-butyl-5-hydroxymethyl-5-nitro-1,3-tetrahydroxazine.

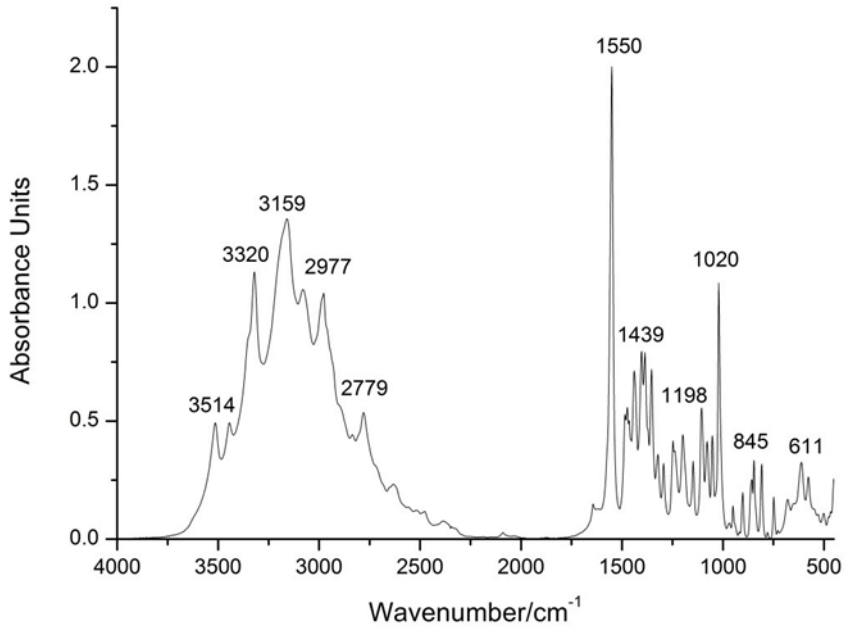


Figure S2. The FTIR spectrum of 2-tertiary-butyl-2-nitro-1,3-propanediol hydrochloride.

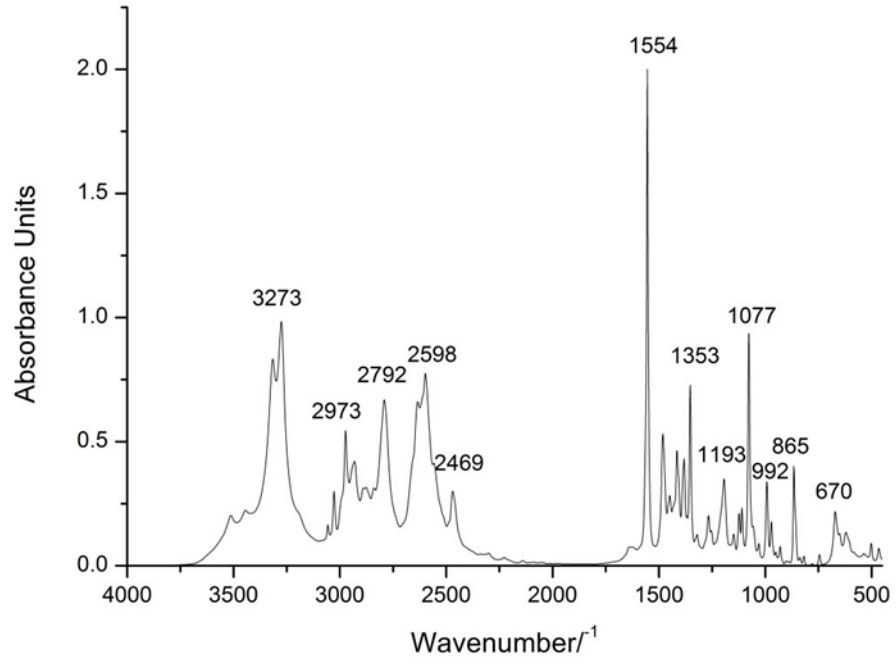


Figure S3. The FTIR spectrum of 1-tertiary-butyl-3-hydroxymethyl-3-nitroazetidine hydrochloride.

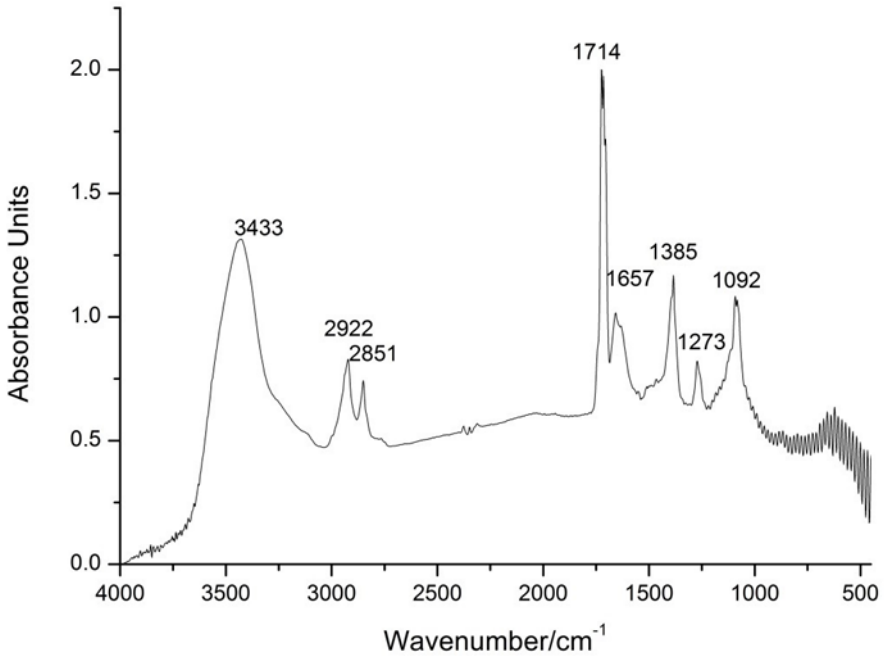


Figure S4. The FTIR spectrum of 1-tertiary-butyl -3,3'-dinitroazetidine.

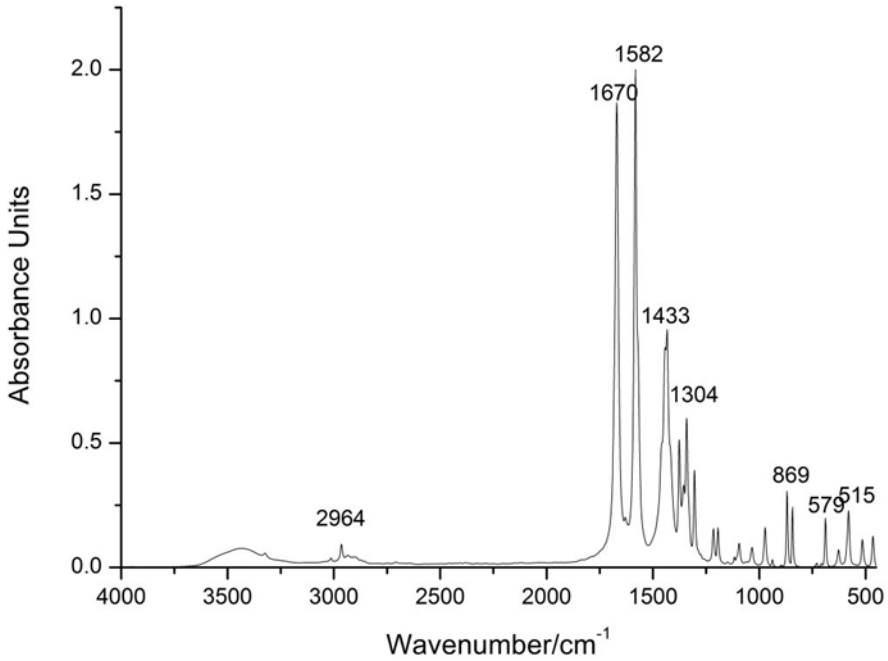


Figure S5. The FTIR spectrum of N-acetyl-3,3'-dinitroazetidine.

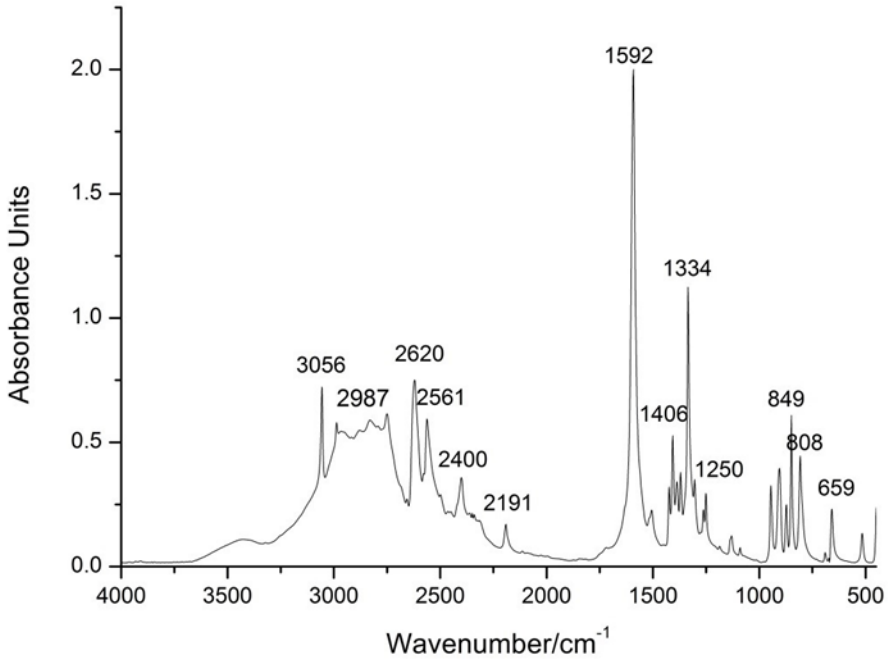


Figure S6. The FTIR spectrum of 3,3'-dinitroazetidine hydrochloride.

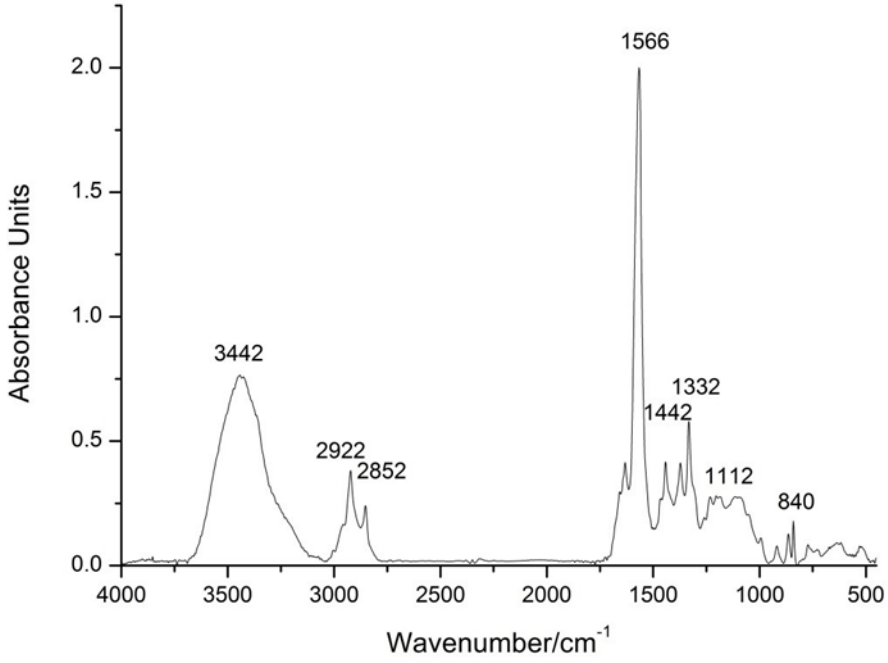


Figure S7. The FTIR spectrum of 3,3'- dinitroazetidine (DNAZ).

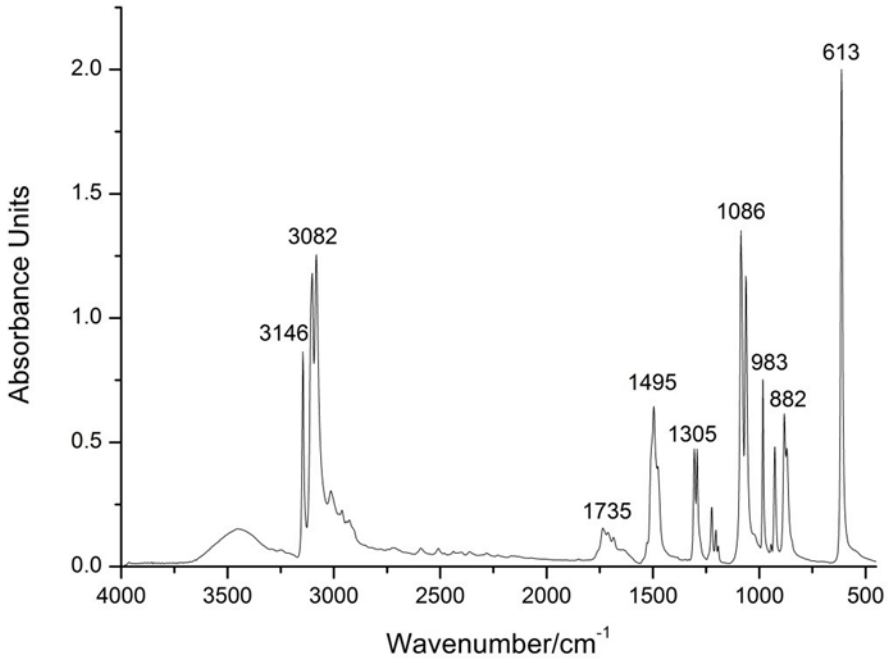


Figure S8. The FTIR spectrum of 4,4'-bi-1,2,4-triazole (BTR).

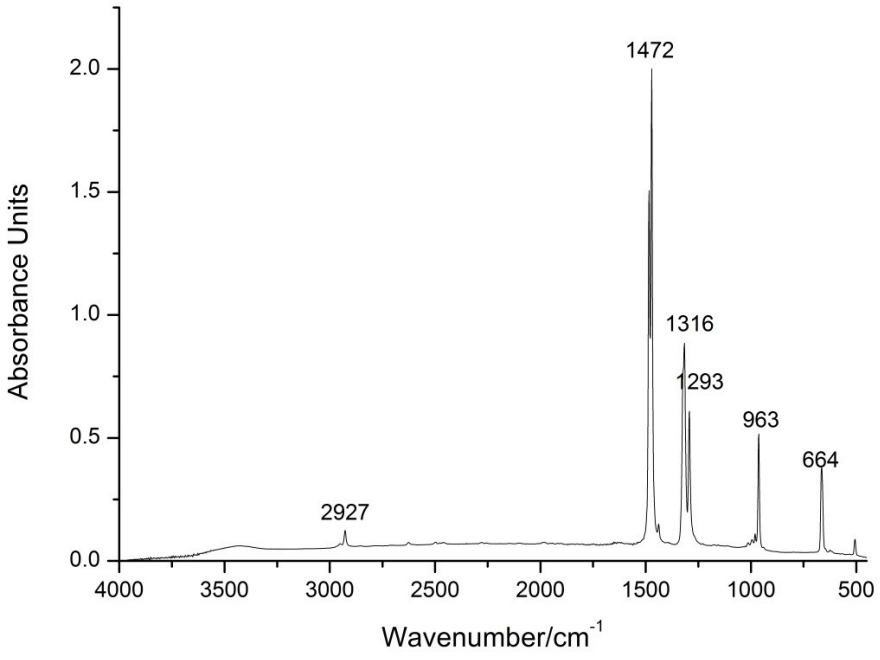


Figure S9. The FTIR spectrum of 3,3',5,5'-tetrachloro-4,4'-bi-1,2,4-triazole (TCBT)

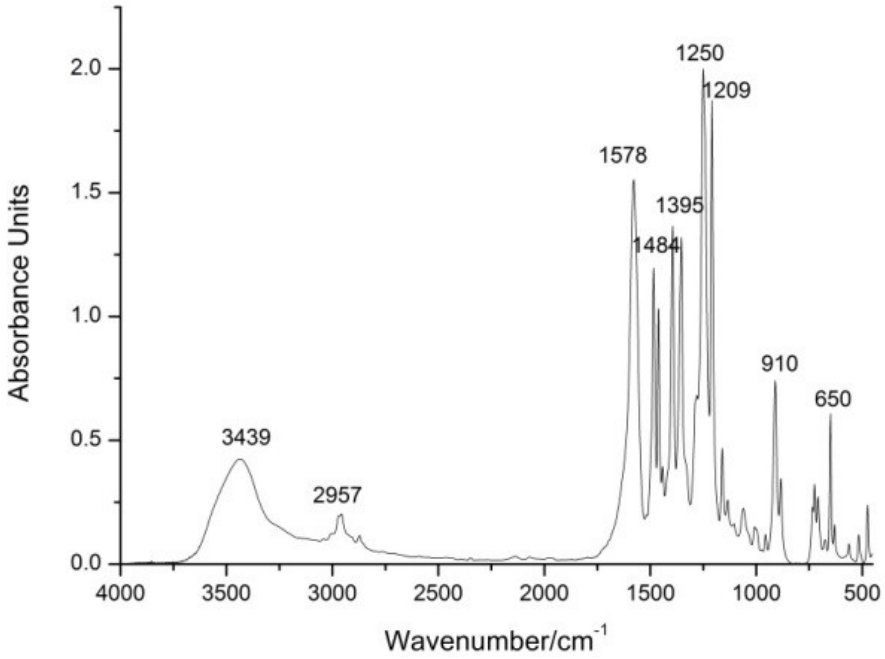


Figure S10. The FTIR spectrum of 5,5'-dichloro-3,3'-bis(3,3'-difluoroazetidine)-4,4'-azo-1,2,4-triazole (**1**)

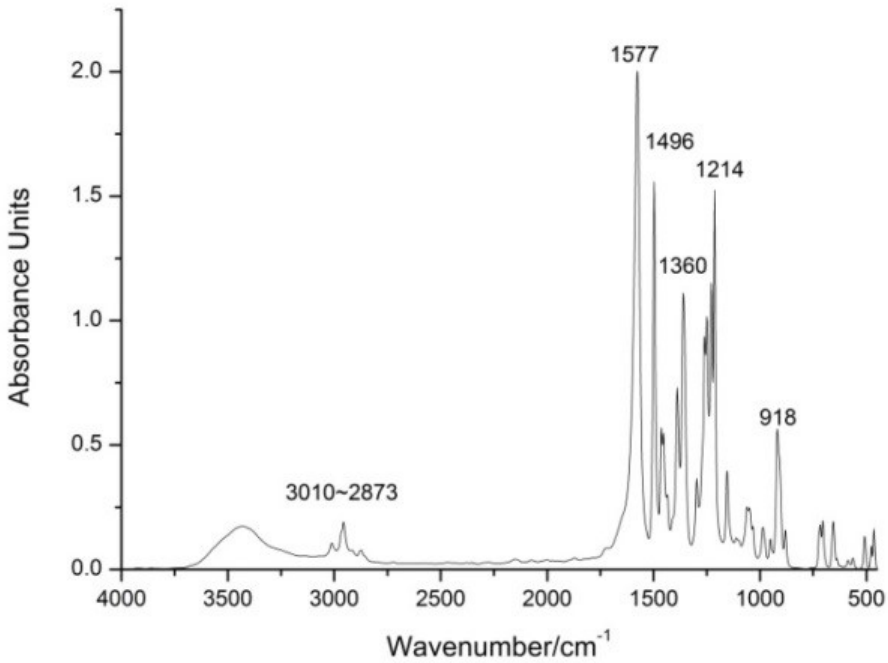


Figure S11. The FTIR spectrum of 5,5'-dichloro-3,3'-bis(3,3'-difluoroazetidine)-4,4'-bi-1,2,4-triazole (**2**)

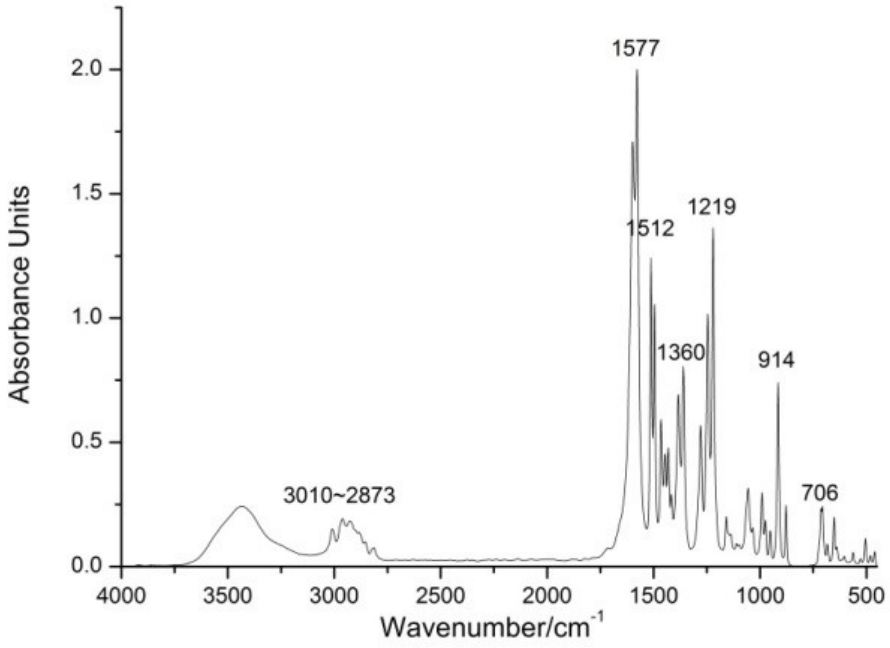


Figure S12. The FTIR spectrum of 5,5'-dichloro-3-(N, N'-dimethyl)-3'-(3,3'-difluoroazetidine)-4,4'-bi-1,2,4-triazole (**3**)

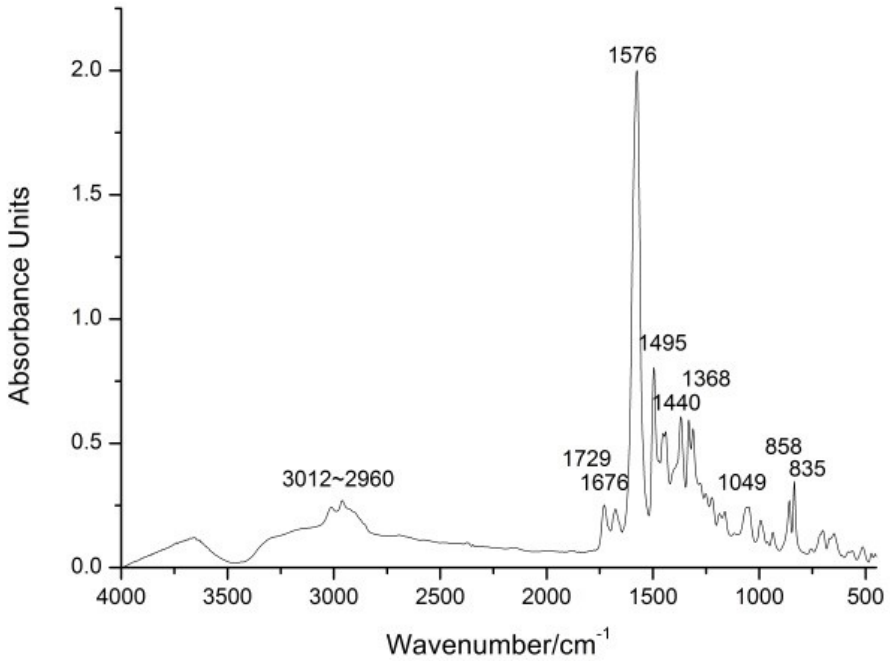


Figure S13. The FTIR spectrum of 5,5'-dichloro-3,3'-bis(3,3'-dinitroazetidine)-4,4'-bi-1,2,4-triazole (**4**)

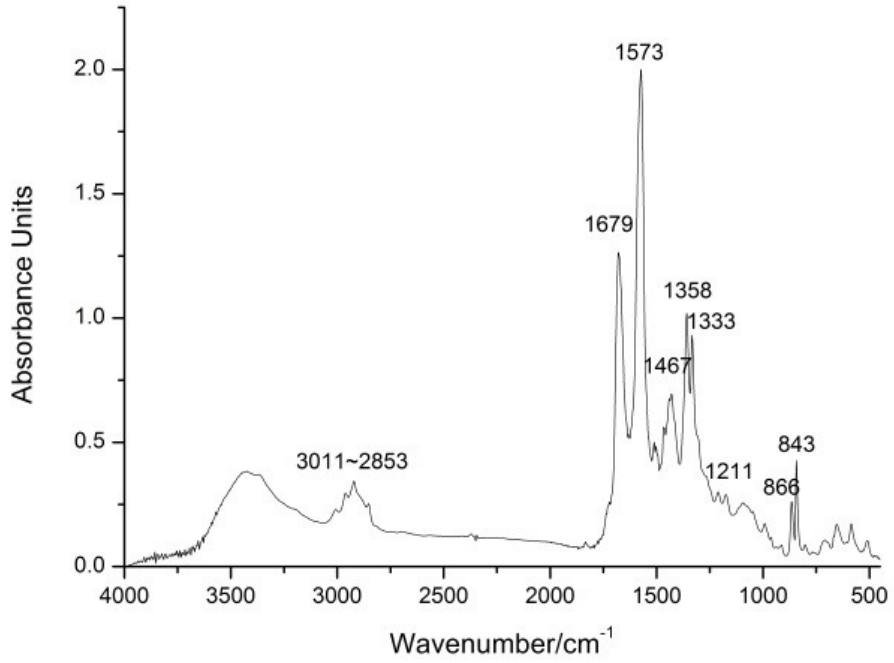


Figure S14. The FTIR spectrum of 5,5'-dichloro-3-(N, N'-dimethyl)-3'-(3,3'-dinitroazetidine)-4,4'-bi-1,2,4-triazole (**5**)

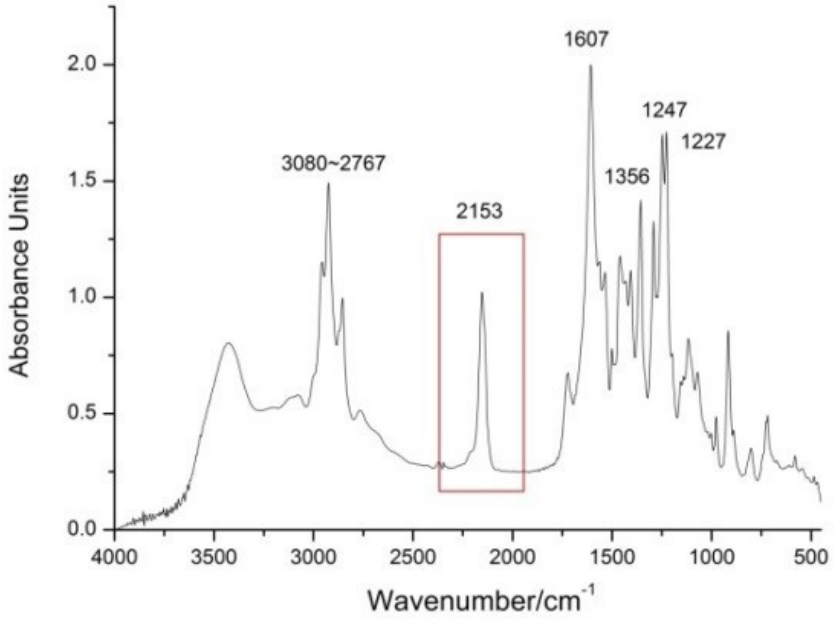


Figure S15. The FTIR spectrum of 5,5'-diazido-3,3'-bis (3,3'-difluoroazetidine)-4,4'-azo-1,2,4-triazole (**6**)

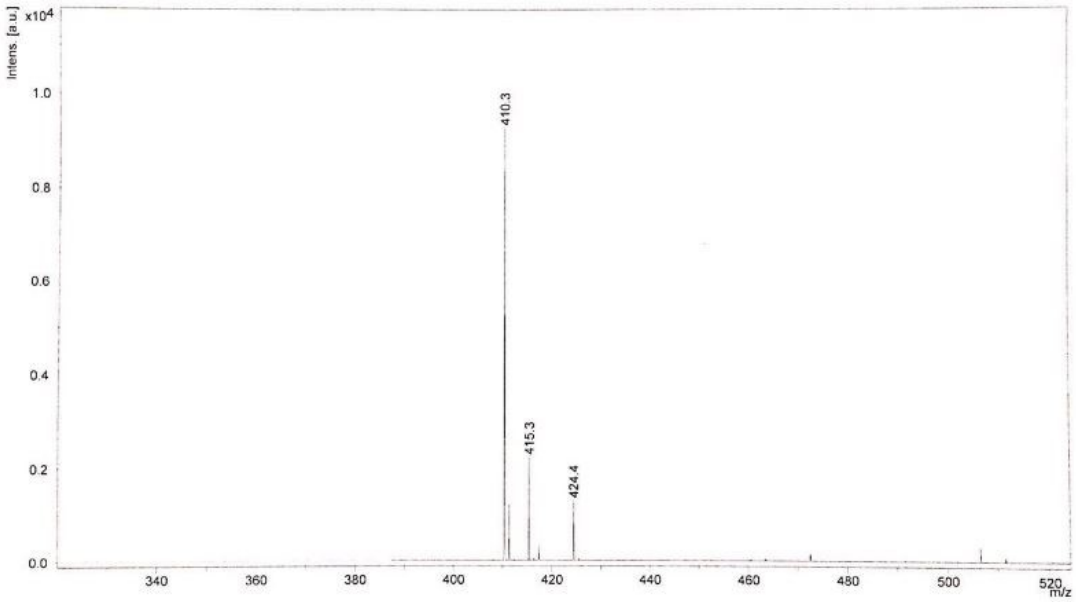


Figure S16. Mass spectrum of 5,5'-dichloro-3,3'-bis(3,3'-difluoroazetidine)-4,4'-azo-1,2,4-triazole (**1**)

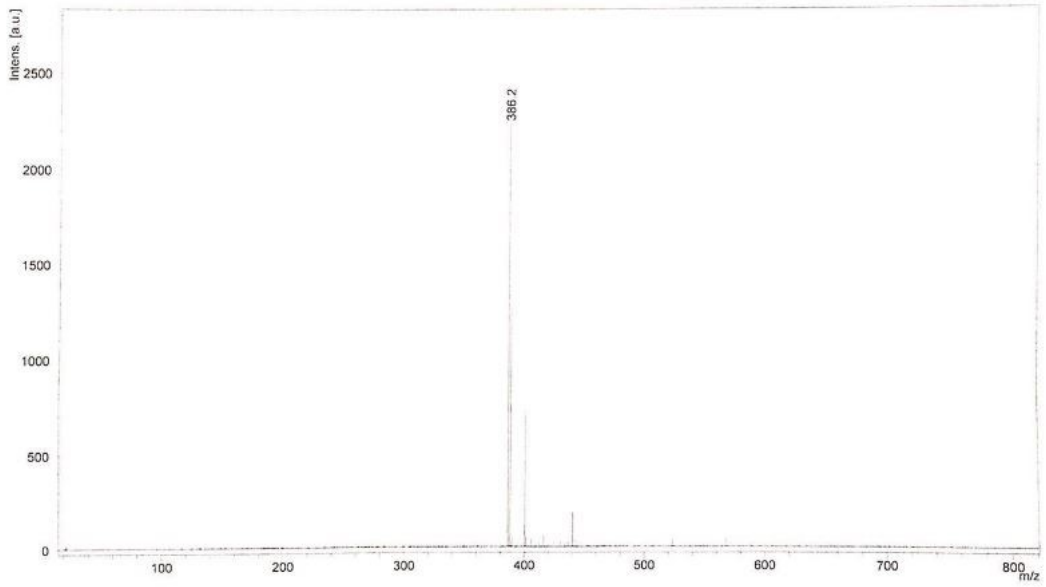


Figure S17. Mass spectrum of 5,5'-dichloro-3,3'-bis(3,3'-difluoroazetidine)-4,4'-bi-1,2,4-triazole (**2**)

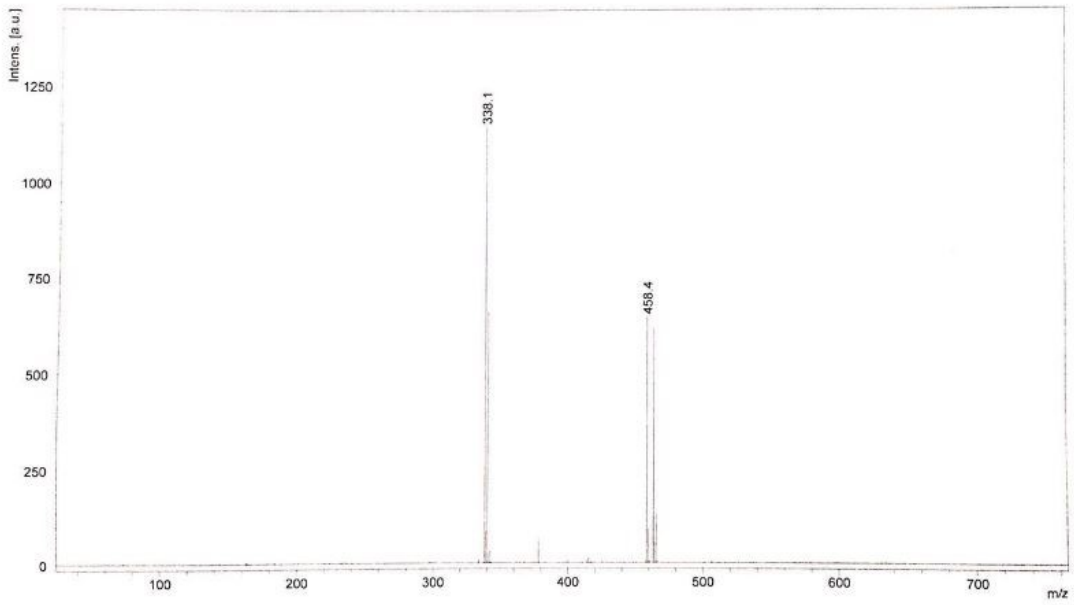


Figure S18. Mass spectrum of 5,5'-dichloro-3-(N, N'-dimethyl)-3'-(3,3'-difluoroazetidine)-4,4'-bi-1,2,4-triazole (**3**)

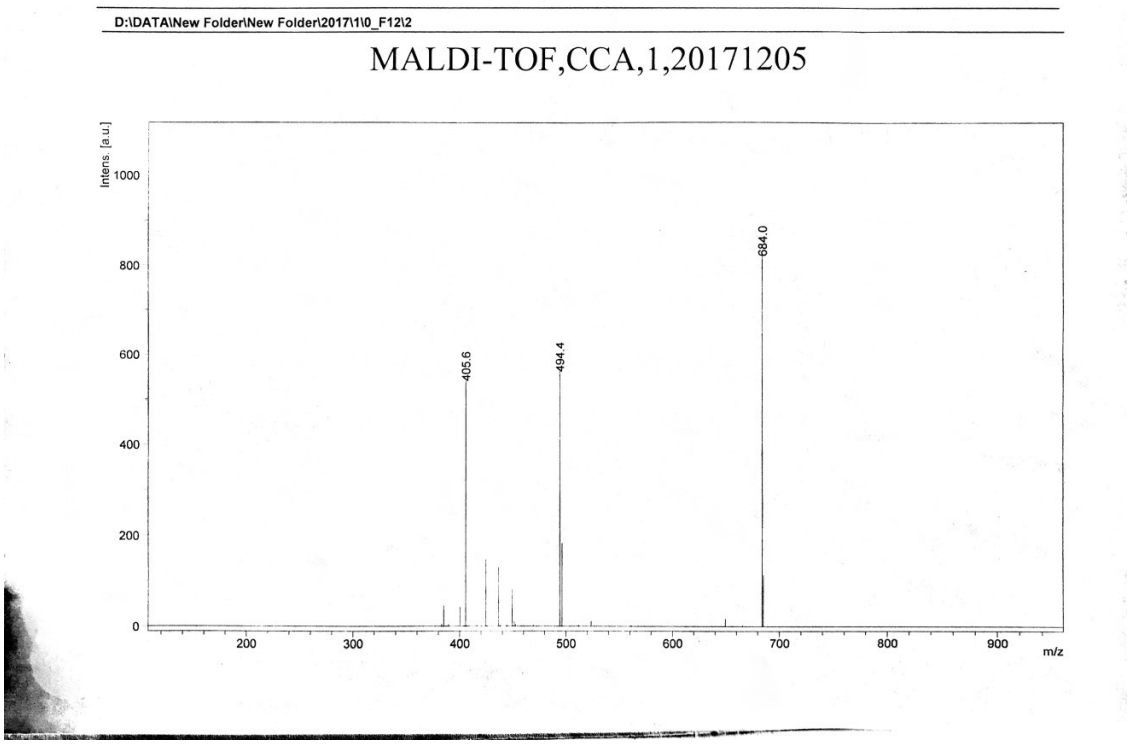


Figure S19. Mass spectrum of 5,5'-dichloro-3,3'-bis(3,3'-dinitroazetidine)-4,4'-bi-1,2,4-triazole (**4**)

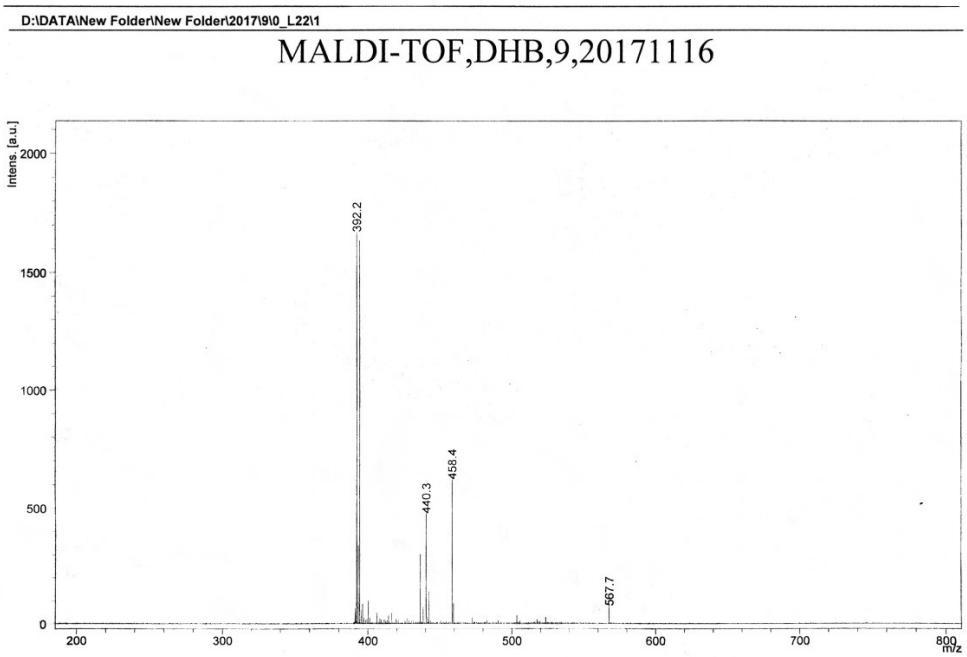


Figure S20. Mass spectrum of 5,5'-dichloro-3-(N, N'-dimethyl)-3'-(3,3'-dinitroazetidine)-4,4'-bi-1,2,4-triazole (**5**)

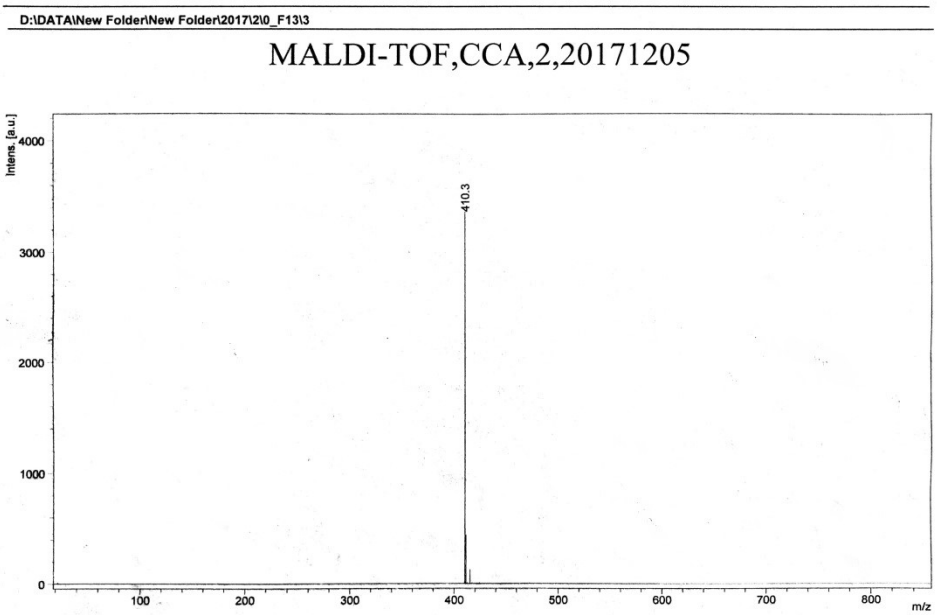


Figure S21. Mass spectrum of 5,5'-diazido-3,3'-bis (3,3'-difluoroazetidine)-4,4'-azo-1,2,4-triazole (**6**)

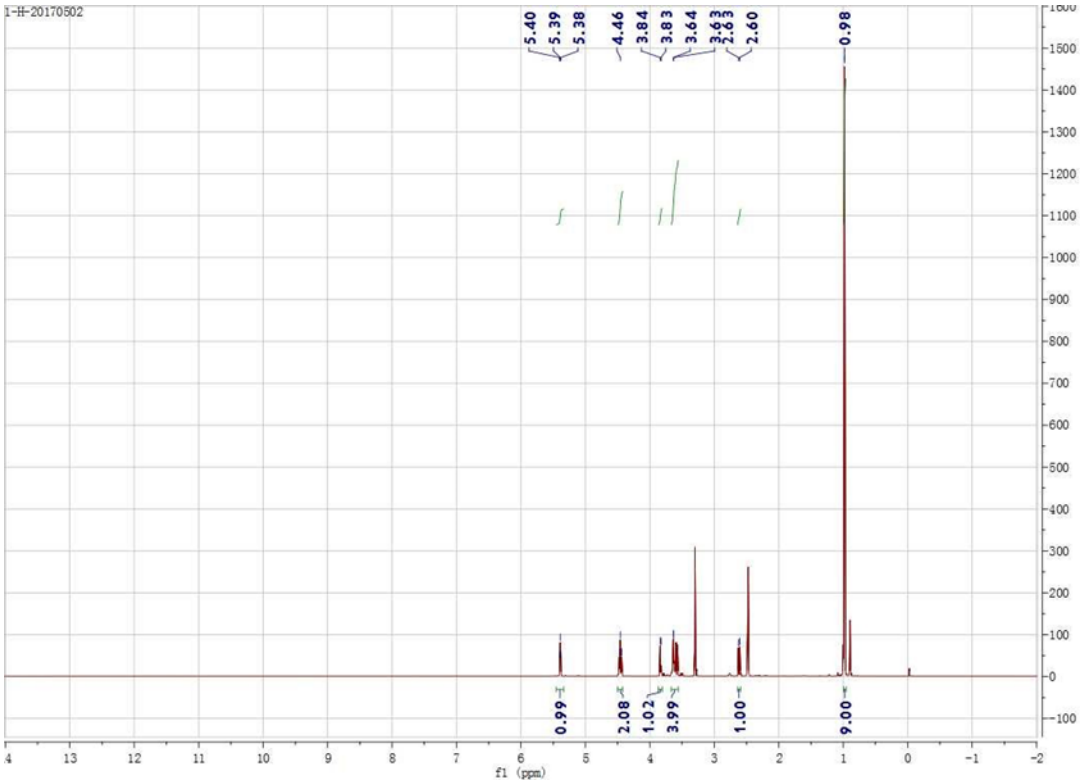


Figure S22. ^{1}H NMR spectrum (400 MHz) of 1-tertiary-butyl-5-hydroxymethyl-5-nitro-1,3-tetrahydroxazine in DMSO-d_6.

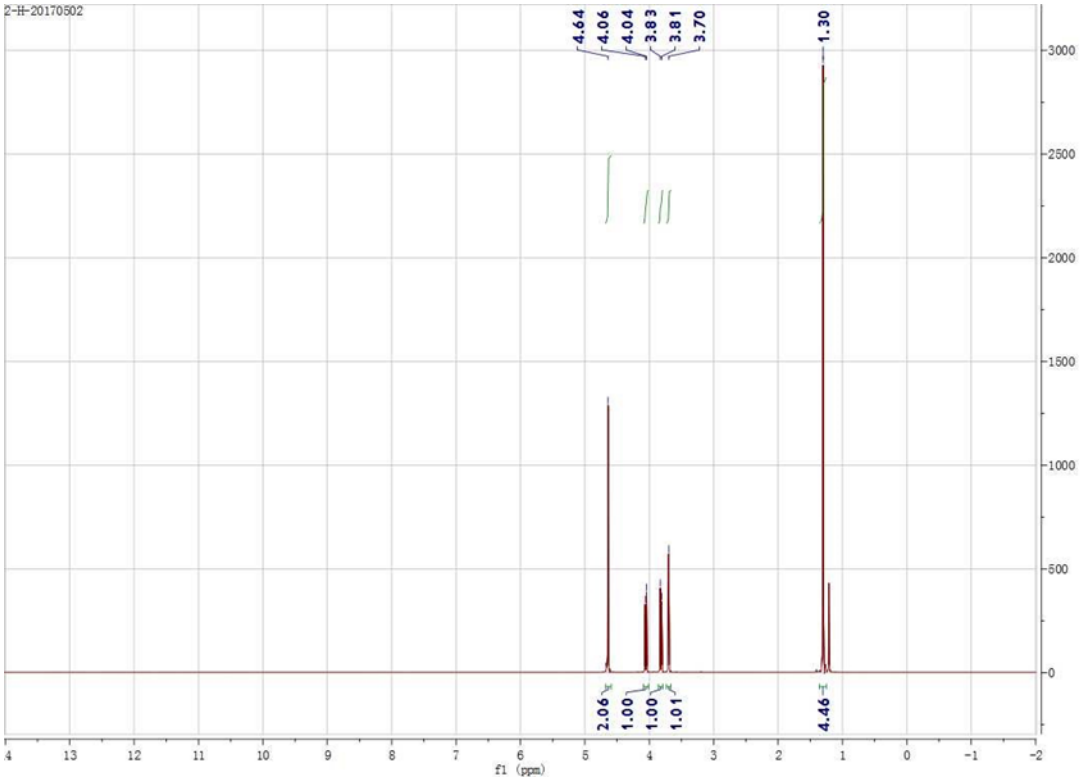


Figure S23. ^{1}H NMR spectrum (400 MHz) of 2-tertiary-butyl-2-nitro-1,3-propanediol hydrochloride in DMSO-d_6.

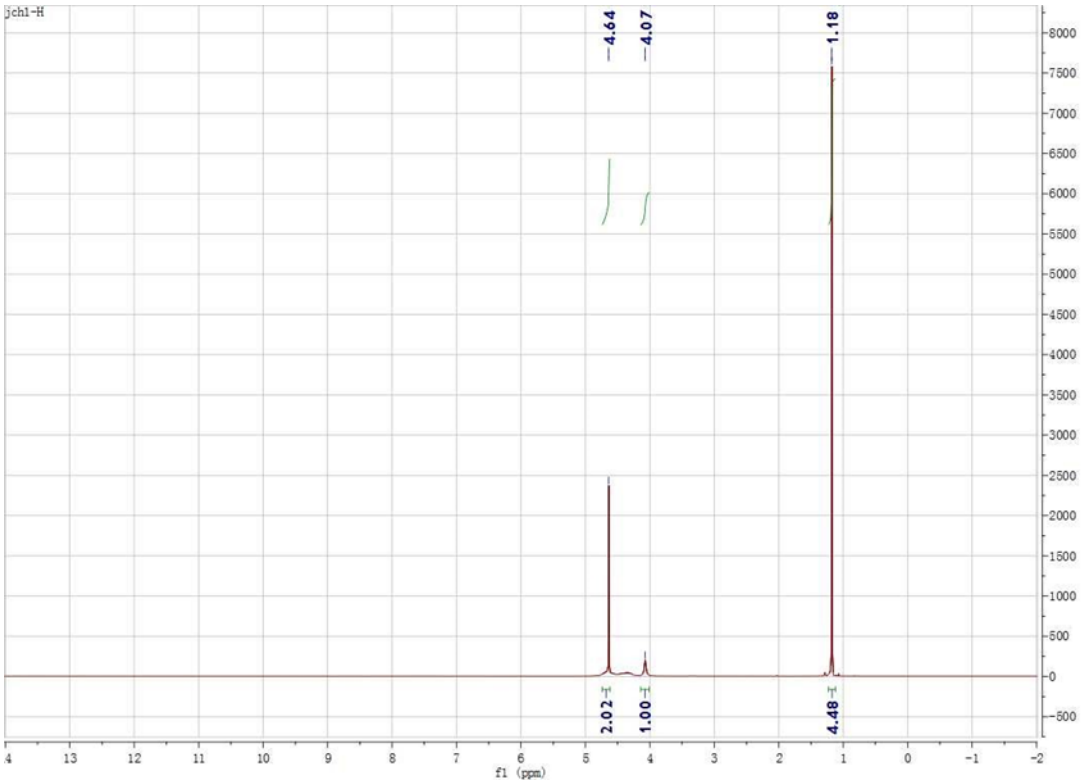


Figure S24. ^{1}H NMR spectrum (400 MHz) of 1-tertiary-butyl-3-hydroxymethyl-3-nitroazetidine hydrochloride in DMSO-d_6.

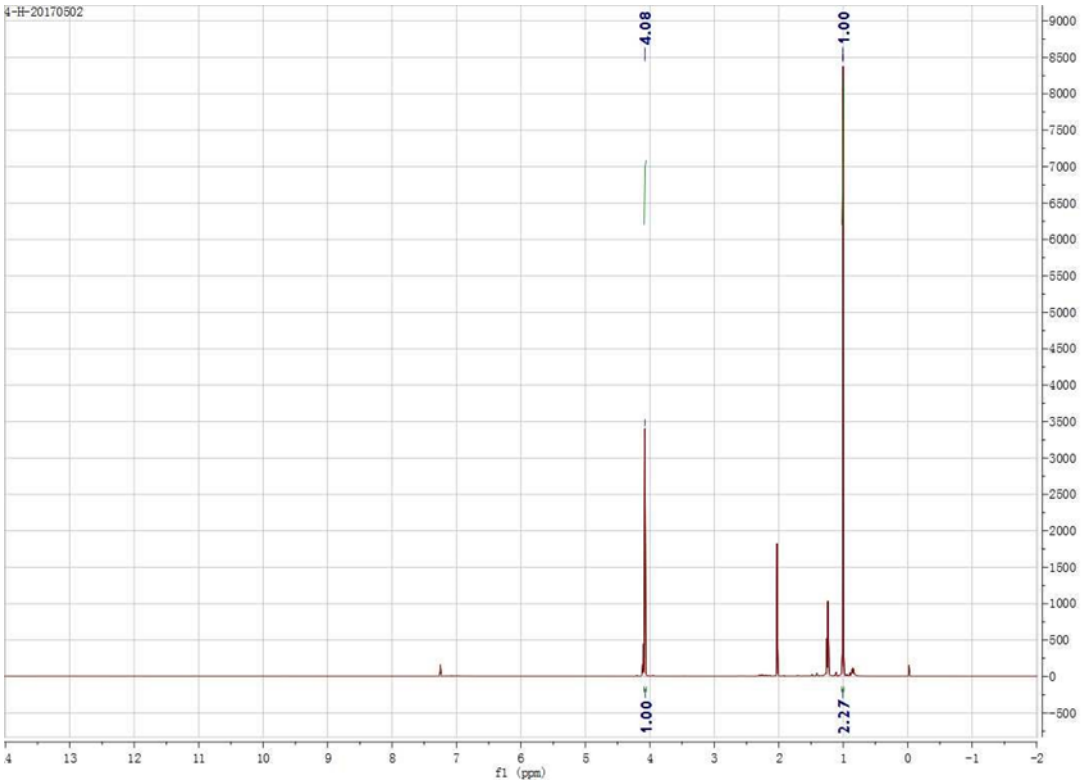


Figure S25. ^{1}H NMR spectrum (400 MHz) of 1-tertiary-butyl -3,3'-dinitroazetidine in DMSO-d_6.

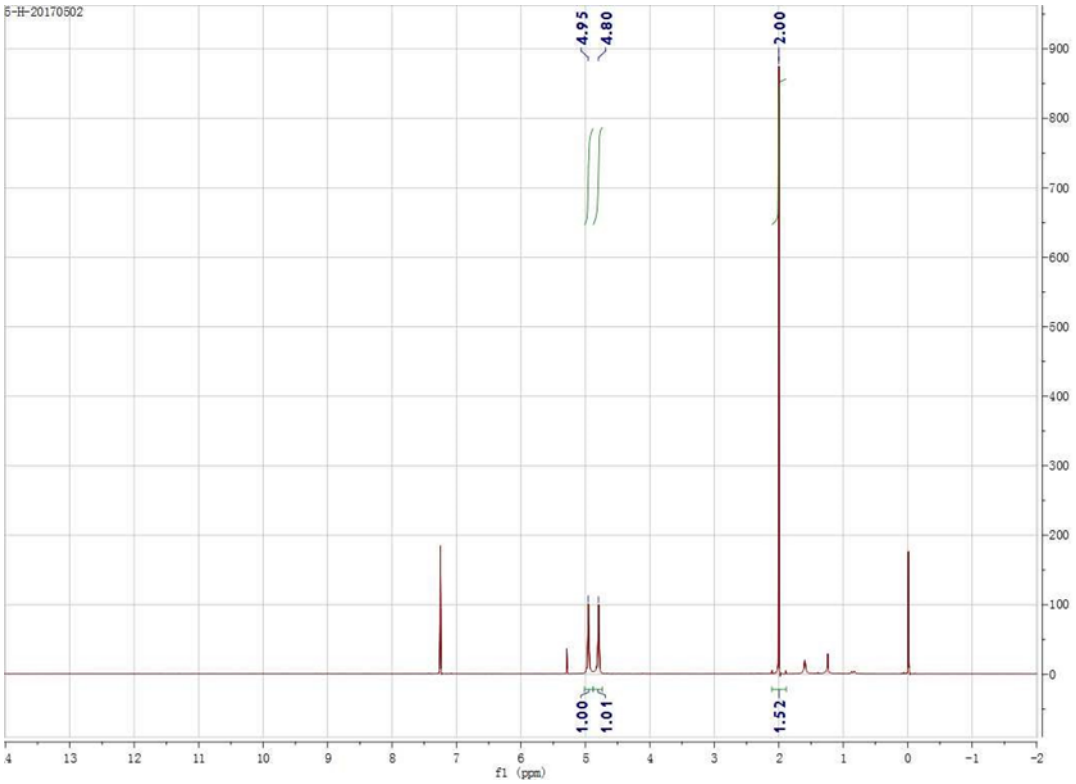


Figure S26. ^{1}H NMR spectrum (400 MHz) of N-acetyl-3,3'-dinitroazetidine in DMSO-d_6.

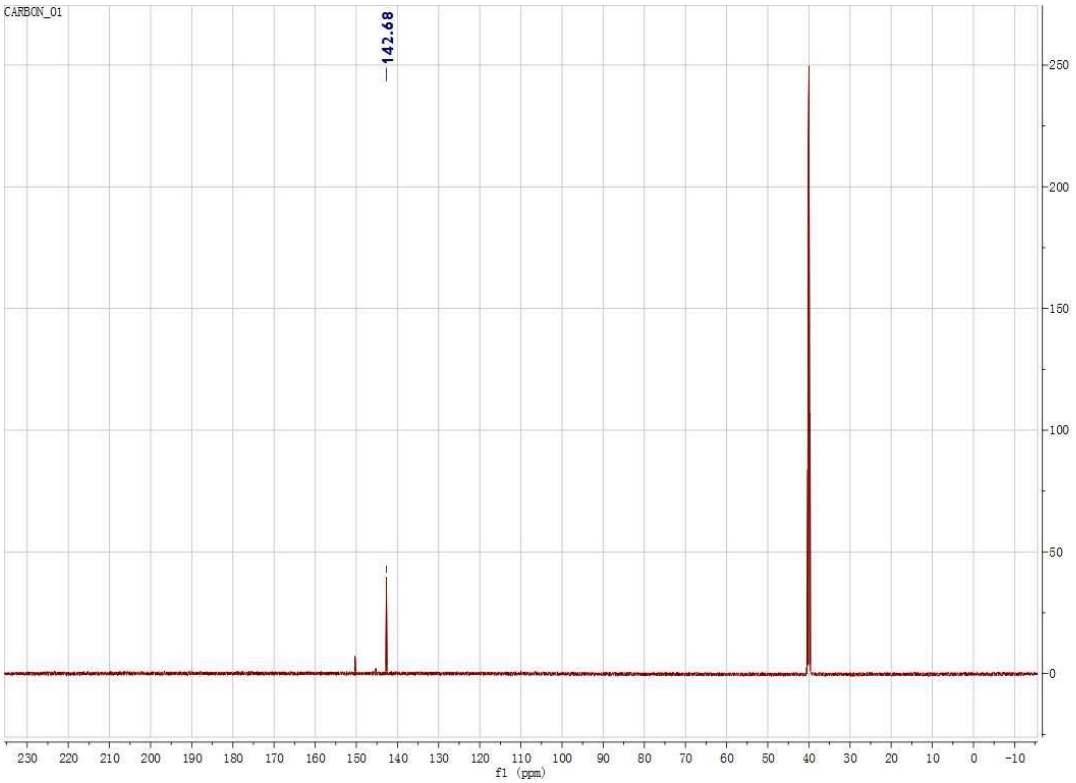


Figure S27. ^{13}C NMR spectrum (100 MHz) of 3,3',5,5'-tetrachloro-4,4'-bi-1,2,4-triazole (**TCBT**) in DMSO-d_6.

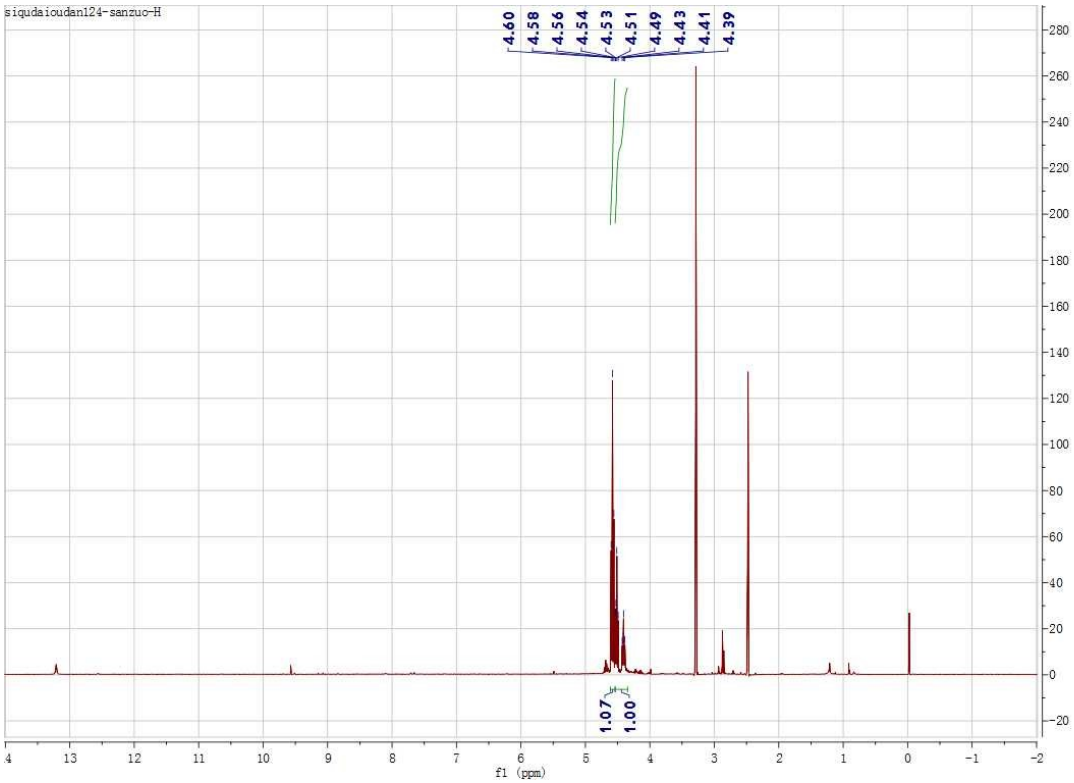


Figure S28. ^{1}H NMR spectrum (400 MHz) of 5,5'-dichloro-3,3'-bis(3,3'-difluoroazetidine)-4,4'-azo-1,2,4-triazole (**1**) in DMSO-d_6.

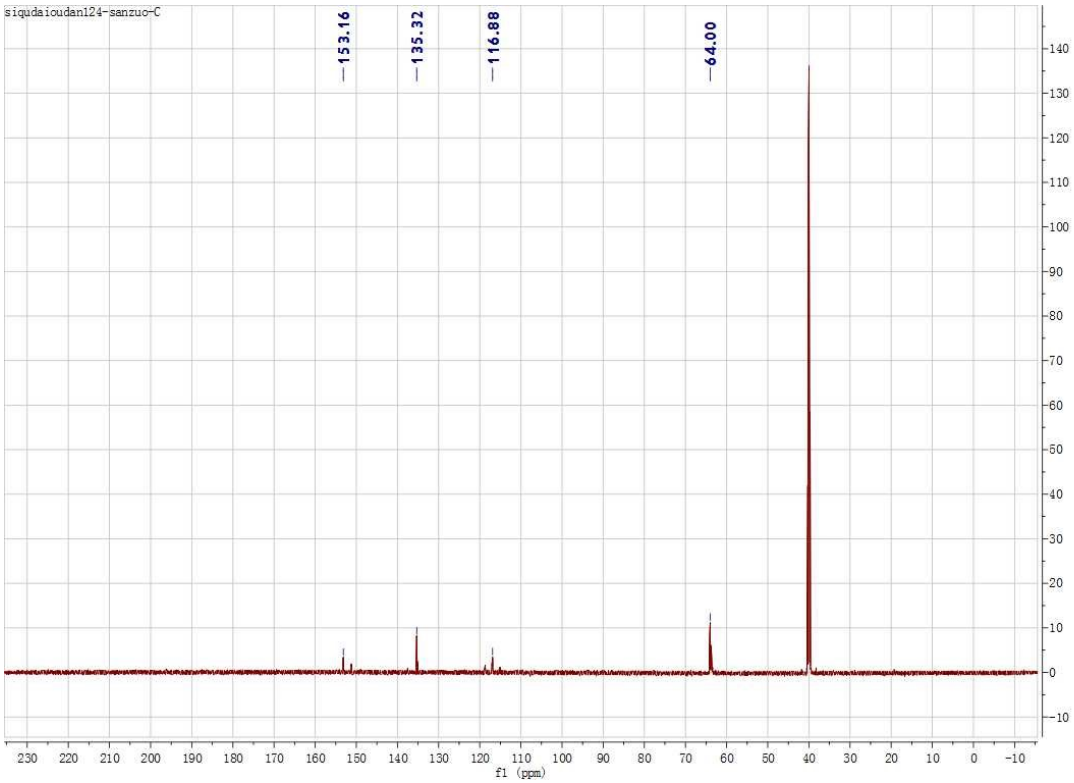


Figure S29. ^{13}C NMR spectrum (100 MHz) of 5,5'-dichloro-3,3'-bis(3,3'-difluoroazetidine)-4,4'-azo-1,2,4-triazole (**1**) in DMSO-d_6.

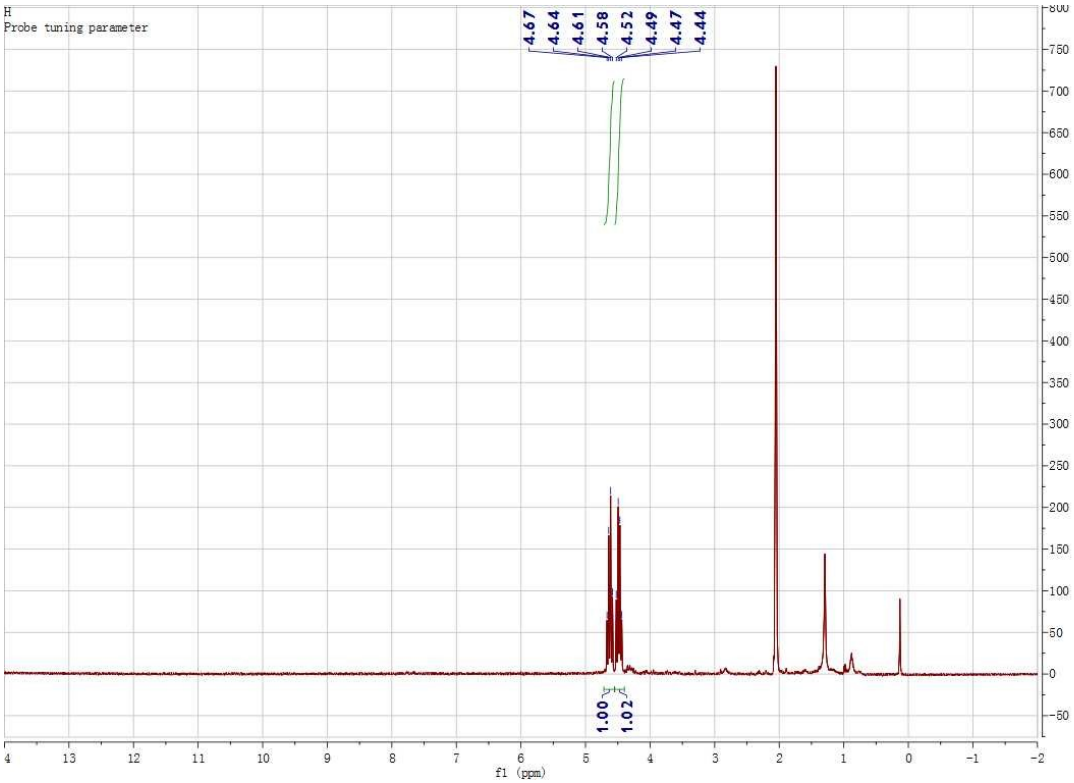


Figure S30.[1]H NMR spectrum (400 MHz) of 5,5'-dichloro-3,3'-bis(3,3'-difluoroazetidine)-4,4'-bi-1,2,4-triazole (**2**) in DMSO-d_6.

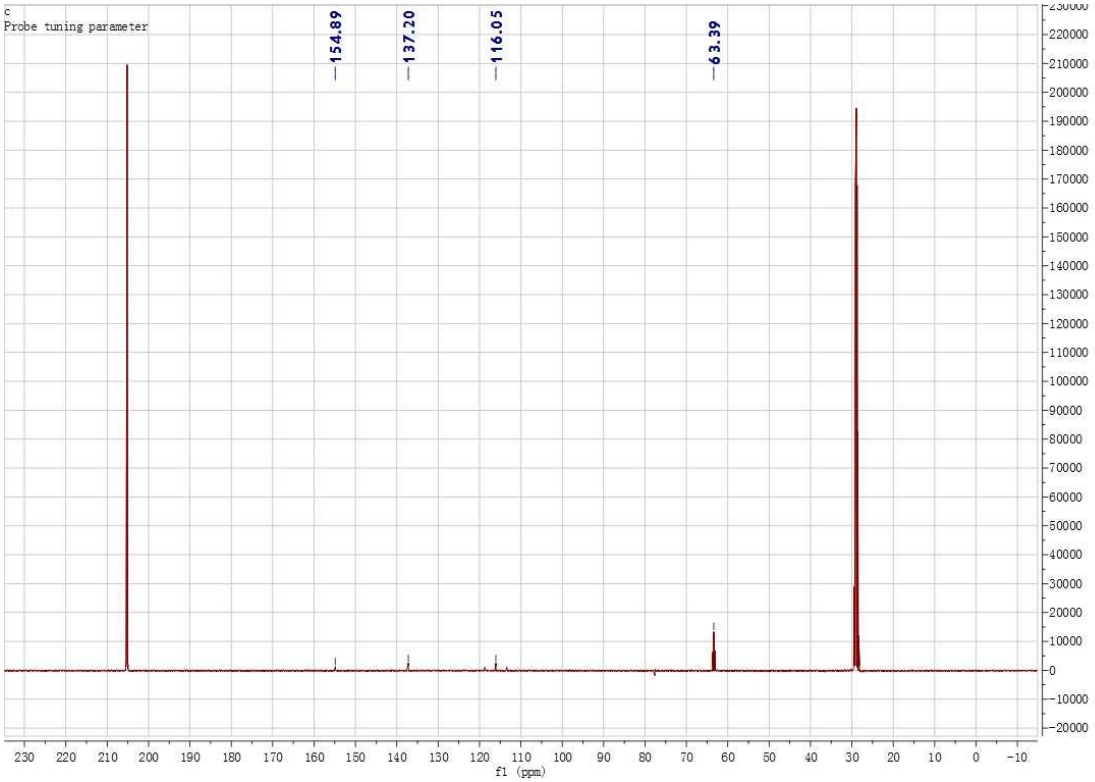


Figure S31.[13]C NMR spectrum (100 MHz) of 5,5'-dichloro-3,3'-bis(3,3'-difluoroazetidine)-4,4'-bi-1,2,4-triazole (**2**) in DMSO-d_6.

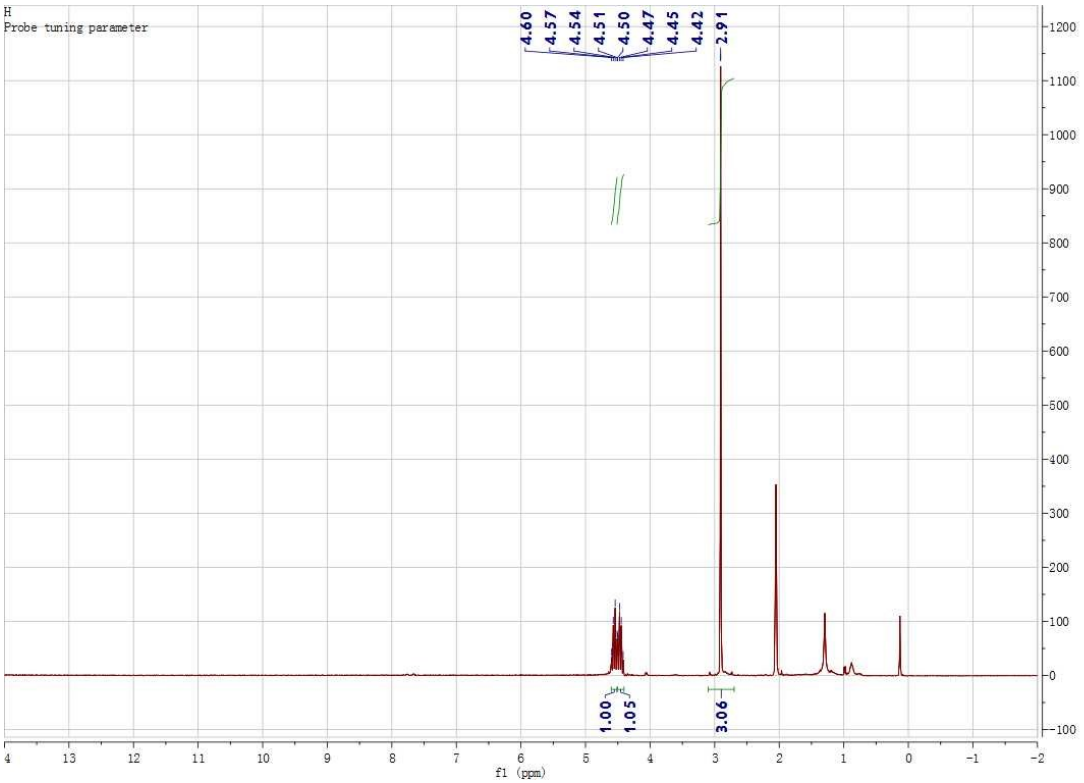


Figure S32.[1]H NMR spectrum (400 MHz) of 5,5'-dichloro-3-(N, N'-dimethyl)-3'-(3,3'-difluoroazetidine)-4,4'-bi-1,2,4-triazole (**3**) in DMSO-d_6.

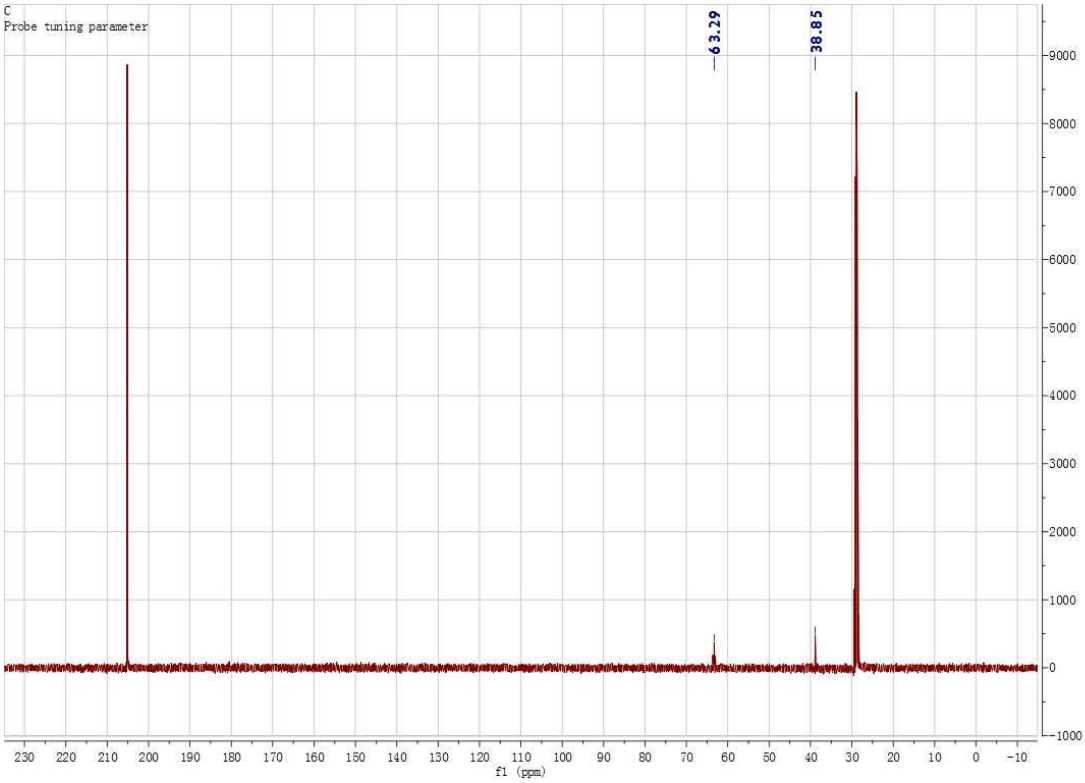


Figure S33.[13]C NMR spectrum (100 MHz) of 5,5'-dichloro-3-(N, N'-dimethyl)-3'-(3,3'-difluoroazetidine)-4,4'-bi-1,2,4-triazole (**3**) in DMSO-d_6.

4. Calculation method for enthalpy of formation.

Enthalpy of formation is one of the most important parameters for energetic compounds. Definition of gas phase enthalpy of formation[4] was used to convert quantum mechanical energies of the most stable simple substance to enthalpy of formation of molecules can be given in terms of (1) at 298 K:

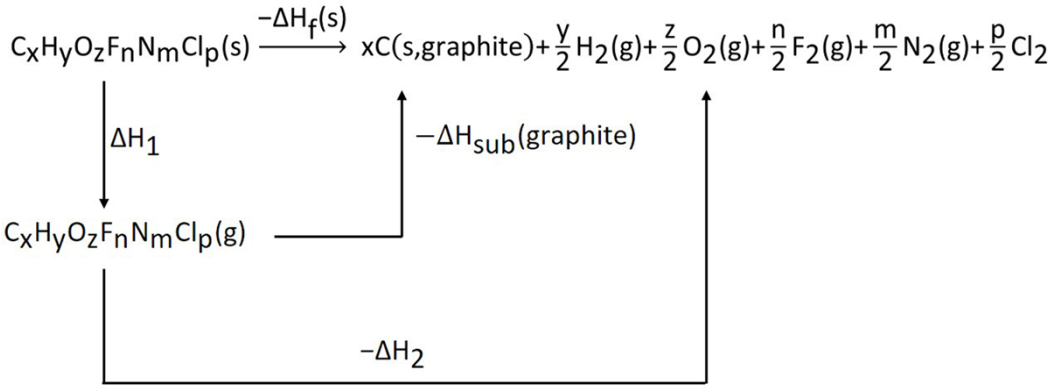


Figure S34. Born-Haber cycle for the formation of the energetic compounds.

$$\Delta H_f(\text{solid, 298 K}) = \Delta H_{sub}(\text{graphite, 298 K}) + \Delta H_2 - \Delta H_1 \quad (1)$$

$$\Delta H_{sub} = 0.000276A^2 + 1.650087\sqrt{v\sigma_{tot}^2} + 2.966078 \quad (2)$$

where A is the surface area of 0.001 e·bohr^{-3} isosurface of the electronic density, the three coefficients were determined by Rice et al.[5] The ν is the degree of balance between positive potential and negative potential on the surface, σ_{tot}^2 is the variance of total electrostatic potential on molecular surface.

5. Cartesian coordinates of compounds (1-6) for electronic structure calculation at M06-2X/6-311G (d, p)[6-7].

Compound **1**

C	1.93804300	1.72490100	-0.25412800
C	0.12326000	2.91117500	0.00678100
N	0.56876800	1.59932300	-0.00798600
N	2.23987700	2.98152100	-0.36556200
N	1.08720800	3.73116400	-0.19757000
N	-0.28951300	0.54381100	-0.03123700
N	0.28947200	-0.54370900	0.03107300
N	-0.56876000	-1.59925600	0.00786200
C	-0.12320000	-2.91110200	-0.00697100
C	-1.93802300	-1.72490200	0.25406700
N	-2.23979600	-2.98153700	0.36550100
N	-1.08709900	-3.73112200	0.19749000
Cl	-1.49810800	3.30714400	0.33673600
Cl	1.49817300	-3.30700100	-0.33700200
C	-3.18940200	0.17236300	-0.75948100
C	-4.19386300	-0.94417900	0.77226300
C	-4.59357700	0.19539700	-0.16031400
H	-3.16798300	-0.38154200	-1.70208300
H	-2.67624700	1.12660800	-0.83346400
H	-4.53893400	-1.91307300	0.40486700
H	-4.41350900	-0.81042900	1.82974300
C	4.19390900	0.94409200	-0.77206500
C	3.18929400	-0.17239200	0.75959000
C	4.59350100	-0.19548800	0.16053900

H	4.53896000	1.91298000	-0.40463500
H	4.41365600	0.81032500	-1.82952300
H	3.16781700	0.38156100	1.70215800
H	2.67615200	-1.12663900	0.83355600
N	-2.78266300	-0.65826200	0.40966400
N	2.78264500	0.65819200	-0.40964000
F	-4.86925800	1.34997300	0.48678900
F	-5.60936500	-0.04809700	-1.00615200
F	5.60923100	0.04795800	1.00646200
F	4.86920900	-1.35008600	-0.48653700

Compound **2**

C	-0.43428300	1.70113700	-1.69747300
C	1.28935000	0.45439900	-1.21365900
C	3.25566200	-1.00550400	-1.16620400
H	4.21610200	-0.50589200	-1.27918300
H	2.90315100	-1.41478800	-2.11573800
C	3.15061700	-2.00762400	-0.01516200
C	1.91392400	-1.26928600	0.50387800
H	0.98781300	-1.80617800	0.28255000
H	1.95607000	-0.95117600	1.54611900
C	0.25754700	1.84560000	1.70026700
C	-0.92179000	0.05730300	1.29546300
C	-2.32070700	-0.85473100	-0.57328800
H	-1.82754200	-1.02014900	-1.53138800
H	-2.89542400	0.07469200	-0.56888900
C	-3.14035300	-2.02514600	-0.02356600

C	-2.39457500	-1.90469200	1.30624300
H	-2.97845400	-1.38512500	2.06960300
H	-1.95251900	-2.81977200	1.69608800
Cl	-1.84008300	2.63037100	-1.46447100
Cl	1.22684400	3.20505700	1.39806000
F	2.95202600	-3.28973800	-0.37230300
F	4.19719900	-1.97941800	0.83420200
F	-2.90989800	-3.18745200	-0.66767200
F	-4.47006200	-1.84030800	0.02309500
N	0.19314700	1.06516400	-0.63641300
N	-0.17271000	1.03013800	0.66458400
N	1.29659100	0.68504100	-2.49205800
N	0.20047500	1.48668500	-2.78932100
N	-0.95253100	0.28219200	2.57193400
N	-0.19403700	1.42121300	2.82314200
N	2.23164900	-0.19428700	-0.47384900
N	-1.43684900	-1.01191300	0.61411600

Compound **3**

C	-1.05650000	-0.49079100	1.80114600
C	-1.74602700	1.19965000	0.59913300
C	-3.16676900	2.84049100	-0.34955000
H	-4.00447700	2.26538600	0.04025400
H	-3.42159400	3.23554600	-1.33318200
H	-2.96344100	3.67105500	0.33639300
C	-0.86606000	2.63075200	-1.14053300
H	-0.61324600	3.56053300	-0.61521400

H	-1.12969600	2.86603000	-2.17195200
H	0.01218100	1.98756500	-1.14426000
C	-1.18028900	-1.36232200	-1.40977300
C	0.79074900	-0.47756000	-1.14940800
C	3.14812200	0.18471800	-1.23558900
H	3.39734100	0.93465400	-1.98395900
H	3.35132900	-0.82571000	-1.59817400
C	3.69270000	0.42376300	0.17283300
C	2.28333800	0.22496500	0.73507400
H	2.15964400	-0.76890100	1.17153700
H	1.91729200	1.00588800	1.40059500
Cl	-0.26110600	-1.94078200	2.20674700
Cl	-2.79800400	-1.74977600	-1.06473300
F	4.62738900	-0.44056600	0.60379400
F	4.17172600	1.67119600	0.36241200
N	-1.83547900	0.20445700	2.53901600
N	-2.27305400	1.28656000	1.78229800
N	-0.89919800	0.09285300	0.55007600
N	-0.45755200	-0.53278800	-0.56822800
N	-0.45383200	-1.75840000	-2.38926500
N	0.80872900	-1.20046500	-2.22636700
N	-2.00570300	1.96749200	-0.50207800
N	1.78922000	0.32454700	-0.66432700

Compound **4**

C	-0.74472300	-1.66143400	1.12147300
C	-2.36135800	-0.33951100	1.75475300

N	-1.73146600	-0.83518200	0.61964000
N	-2.00427400	-0.50171800	-0.66409600
C	-1.49892700	0.58213600	-1.35345300
C	-3.04574700	-0.94523100	-1.46813700
N	-1.82962300	-0.82299100	2.81429900
N	-0.79638200	-1.65852000	2.41879200
N	-2.12894700	0.73581200	-2.47295500
N	-3.11454900	-0.24407500	-2.53993500
Cl	-3.64072400	0.77156600	1.62386500
Cl	-4.03044700	-2.24044500	-0.99222600
C	0.16035100	2.40777800	-1.61790800
C	-0.18553600	1.84377900	0.42070800
C	0.77519500	2.81064700	-0.27742500
H	-0.61489200	3.11051600	-1.93958400
H	0.85808700	2.18533900	-2.42183300
H	-1.06174100	2.37884900	0.79861800
H	0.24713300	1.18942200	1.17893300
C	0.91979400	-1.76980700	-0.73400900
C	1.30491800	-2.93342100	1.02829900
C	2.18099300	-2.16998600	0.03099500
H	0.79779900	-0.69306800	-0.85274900
H	0.82445400	-2.28725700	-1.68745200
H	1.39213600	-2.60720100	2.06430700
H	1.40242300	-4.01409600	0.94046500
N	-0.37790800	1.23311000	-0.91741400
N	0.10084500	-2.40500700	0.33791100

N	3.22142600	-2.94879400	-0.71137200
O	3.38802200	-2.64680200	-1.86570300
O	3.80019700	-3.79550500	-0.07932600
N	2.87073300	-0.97312000	0.65270400
O	4.04846100	-0.84564100	0.49650100
O	2.12626300	-0.23923600	1.26785700
N	2.21452500	2.36710900	-0.10048000
O	2.61062100	1.51248500	-0.85552300
O	2.80513900	2.86115100	0.81896600
N	0.72227700	4.26378800	0.07437200
O	0.06774200	4.58174900	1.03241500
O	1.34207500	4.98253300	-0.66901400

Compound **5**

C	2.31025100	-1.28600000	-0.65629200
C	1.65489000	0.46002400	-1.80064000
N	1.54355000	-0.12521000	-0.54302100
N	1.23188600	0.52869300	0.60319300
C	0.02003500	0.59098800	1.25023200
C	2.05468000	1.34330600	1.36387900
N	2.32985800	-0.27999100	-2.59398200
N	2.74347300	-1.39714900	-1.87485800
N	0.10998700	1.35180700	2.29490900
N	1.41350100	1.82602700	2.36523800
Cl	0.93339200	1.96607100	-2.13506300
Cl	3.66841300	1.60974600	0.91283400
C	-2.37141600	0.15805400	1.48013200

C	-1.62844000	-0.07724800	-0.51114400
C	-3.02066600	-0.11486400	0.12079000
H	-2.45450000	1.20741800	1.77282200
H	-2.67294100	-0.50910500	2.28401100
H	-1.44709000	0.88100500	-1.00230000
H	-1.38772400	-0.91905500	-1.15758000
N	-1.06655900	-0.15553900	0.86118300
N	2.59587500	-2.08169400	0.41773700
N	-3.72140400	-1.44716600	0.01140800
O	-4.33756900	-1.80864700	0.98004300
O	-3.61806600	-2.01510100	-1.04583300
N	-3.99210700	0.93601600	-0.36674900
O	-3.54893300	2.05783300	-0.39374600
O	-5.09806200	0.57998400	-0.67096700
C	3.66546600	-3.04533400	0.16540100
H	4.50540000	-2.53863600	-0.30551100
H	3.97857000	-3.45891800	1.12411200
H	3.33355700	-3.85655700	-0.49271600
C	1.46316700	-2.65737300	1.14605500
H	1.05844700	-3.52909100	0.61607800
H	1.80645200	-2.97062700	2.13199600
H	0.66599000	-1.92774600	1.27511400

Compound **6**

C	-1.63472900	2.00478600	-0.25713500
C	0.31911900	2.88626700	0.16959500
N	-0.31896000	1.66480700	0.08487100

N	-1.73418300	3.29408400	-0.34138700
N	-0.49447100	3.85444200	-0.07301600
N	0.37037000	0.49305200	0.11809600
N	-0.37054600	-0.49309300	0.11820400
N	0.31885900	-1.66482000	0.08501200
C	-0.31905600	-2.88633700	0.16972700
C	1.63465100	-2.00461100	-0.25717000
N	1.73412900	-3.29388500	-0.34188600
N	0.49450600	-3.85439400	-0.07345200
C	3.22673400	-0.21943900	0.49500000
C	3.93418200	-1.63984400	-0.95529200
C	4.58289300	-0.53170000	-0.13322600
H	3.14464400	-0.63381700	1.50352700
H	2.90264300	0.81696700	0.45326400
H	4.12795200	-2.62991900	-0.53753200
H	4.11043200	-1.61468200	-2.02907500
C	-3.22676300	0.21959300	0.49493600
C	-3.93436100	1.64018100	-0.95505500
C	-4.58293000	0.53175300	-0.13328200
H	-3.14473800	0.63397900	1.50346200
H	-2.90260000	-0.81677900	0.45314400
H	-4.12812900	2.63010100	-0.53692000
H	-4.11067100	1.61538700	-2.02883300
N	2.61468700	-1.09254900	-0.54917500
N	-2.61479800	1.09279200	-0.54920900
F	5.07456200	0.48387500	-0.87756900

F	5.55577300	-0.91479700	0.71572200
F	-5.55595700	0.91445700	0.71567800
F	-5.07434600	-0.48373000	-0.87793400
N	1.66422600	2.93196800	0.50631500
N	2.11738000	4.09309700	0.53811600
N	2.62602900	5.08223400	0.59534500
N	-1.66409100	-2.93223300	0.50676300
N	-2.11717900	-4.09339900	0.53822400
N	-2.62571000	-5.08258600	0.59536700

References

1. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H., OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* **2009,** *42* (2), 339-341.
2. Sheldrick, M., SHELXS-97, Program for crystal structure solution. *Acta Crystallogr. Sect. A.* **1990,** *46*, 467-473.
3. Politzer, P.; Martinez, J.; Murray, J. S.; Concha, M. C.; Toro-Labbe, A., An electrostatic interaction correction for improved crystal density prediction. *Mol. Phys.* **2009,** *107* (19), 2095-2101.
4. Atkins, P.; Paula, J. D., *Physical chemistry thermodynamics, structure, and change*. 10 ed.; WH Freeman and Company: New York, 2014.
5. Politzer, P.; Ma, Y.; Lane, P.; Concha, M. C., Computational prediction of standard gas, liquid, and solid-phase heats of formation and heats of vaporization and sublimation. *Int. J. Quantum Chem* **2005,** *105* (4), 341-347.
6. Zhao, Y.; Truhlar, D. G., The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* **2007,** *120* (1-3), 215-241.
7. Wong, M. W.; Gill, P. M. W.; Nobes, R. H.; Radom, L., 6-311G(MC)(d,p): a second-row analogue of the 6-311G(d,p) basis set: calculated heats of formation for second-row hydrides. *J. Phys. Chem.* **2002,** *92* (17), 4875-4880.