Supporting Information

Polynitramino Compounds Outperform PETN

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Safety Precautions: While we have experienced no difficulties with the shock instability of the polynitramino compounds **4–7** and polyazide compounds **10**,[1a,b] **18**,[1c] **23**,[1b,e] and **28**,[1b,e] they must be synthesized only in millimole amounts. Manipulations must be carried out in a hood behind a safety shield. Leather gloves must be worn.

General Methods.

^{1}H, ^{13}C and ^{15}N NMR spectra were recorded on a 300 MHz (Bruker AVANCE 300) and 500 MHz (Bruker AVANCE 500) Nuclear Magnetic Resonance spectrometer operating at 300.13, 75.48 and 50.69 MHz, respectively, by using DMSO[D$_6$] or $CDCl_3$ as solvent and locking solvent unless otherwise stated. The melting and decomposition points were obtained on a Differential Scanning Calorimeter (TA Instruments Company, Model: Q10) at a scan rate of 10 °C min^{-1}. IR spectra were recorded using KBr pellets for solids on BIORAD model 3000 FTS spectrometer. Densities of the polynitramines were obtained at room temperature by employing a Micromeritics Accupyc 1330 gas pycnometer. Elemental analyses were determined using an Exeter CE-440 elemental analyzer. Single crystal X-ray diffraction analysis data were collected on a Bruker three-circle platform diffractometer equipped with a SMART PLATINUM 135 CCD detector. Because they were hygroscopic, elemental analysis for polyamino compounds **11**, **19**, **24** and **29** were not successful.

General Procedure

− Hydrogenation

A solution of 12 mmol polyazide (Compound **18** should not be dried.) in 150 mL methanol (3.0 g) containing 5% palladium on carbon (this commercial Pd/C has included 50% water for safety, for 10% Pd/C 1.5 g) was exposed to hydrogen (hydrogen should be replenished two or three times in two weeks) at room temperature for two weeks. After filtration the reaction mixture was checked by NMR, and this showed that the reaction had gone to completion. The filtrate was evaporated in vacuo to yield the polyamine as a colorless oil which was not purified further.

− Synthesis of polyurethane

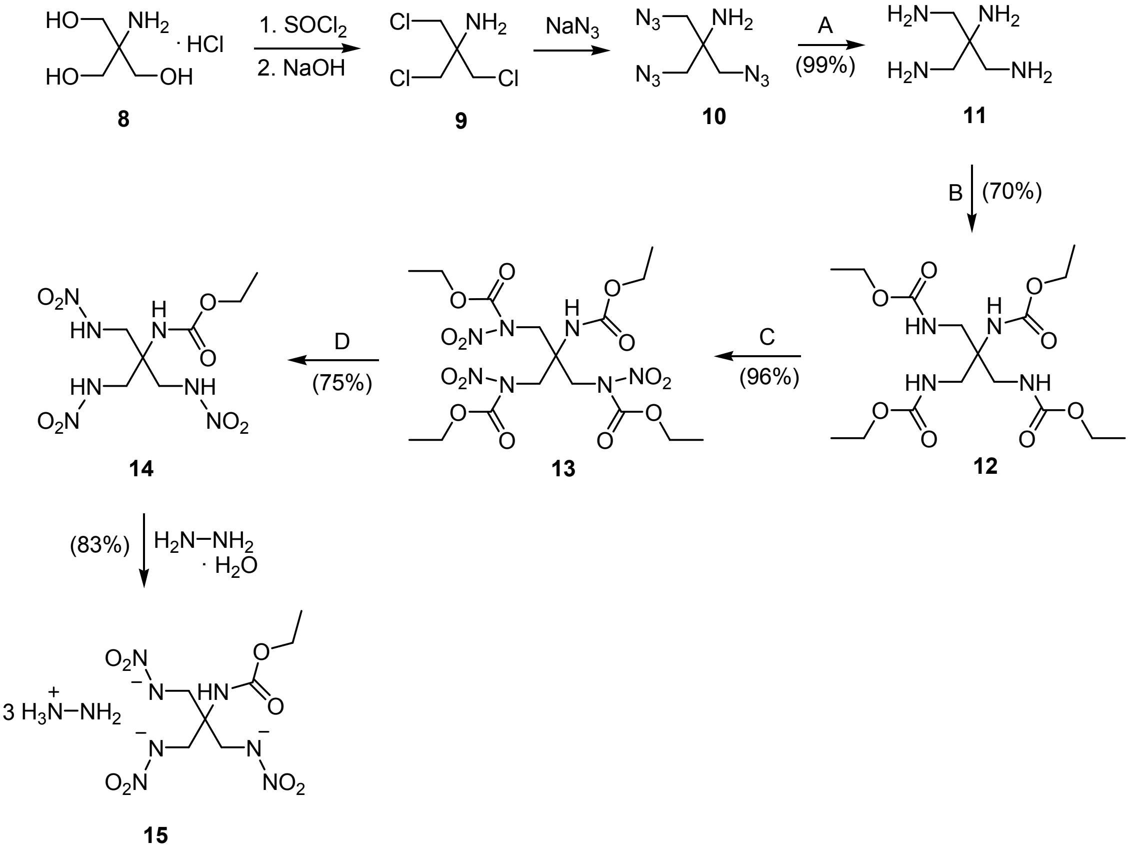
To a solution of 20 mmol polyamine in 100 mL water were dropped ethyl chloroformate [70 mmol for triamine, 90 mmol for tetraamine, 135 mmol for hexaamine, 175 mmol for octaamine] and 50 mL of an aqueous solution containing sodium hydroxide [60 mmol for triamine, 80 mmol for tetraamine, 120 mmol for hexaamine, 160 mmol for octaamine] at the same time under −5 °C. 10 drops ethyl chloroformate was added slowly to the stirred solution in the flask, and then the reminder was added simultaneously with the sodium hydroxide solution at such a rate that the temperature did not rise above 5 °C in an ice/sodium chloride salt bath. After the mixture had been stirred for another 15 hours, the white solid polyurethane was collected on a filter and washed with water. The polyurethane was dissolved in 500 mL ethyl acetate and washed five times (300 mL x 5) with water. The organic layer was dried with magnesium sulfate. After removal of the solvent in vacuo, the pure white solid remained.

− Synthesis of polynitrourethane

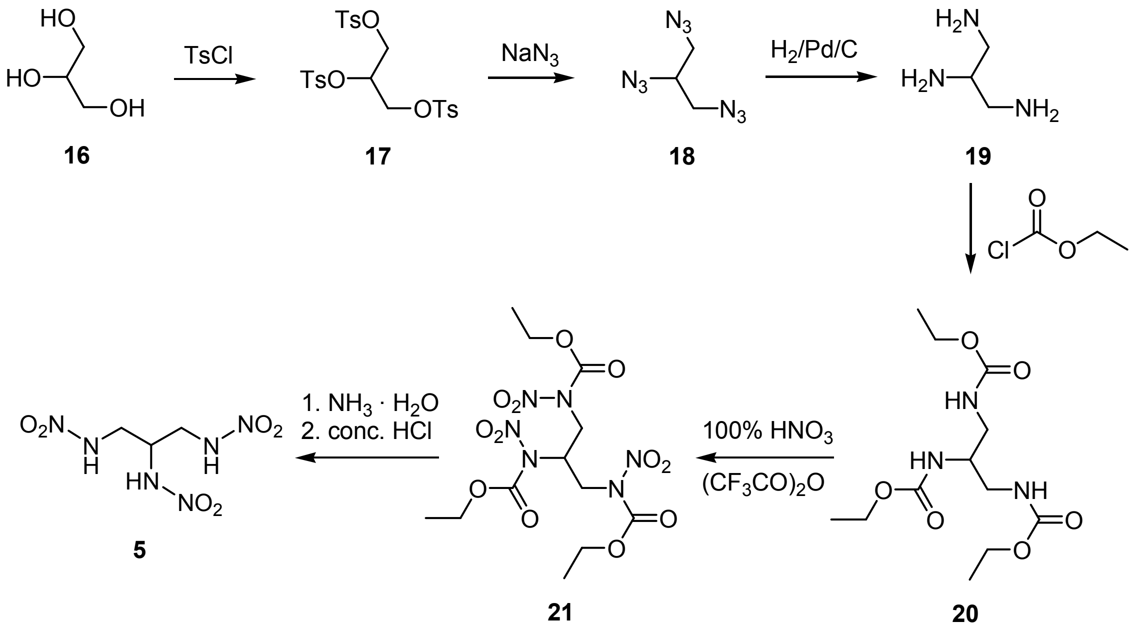
To a mixture of 20 mL 100% nitric acid and 10 mL trifluoroacetic anhydride was added slowly 10 mmol polyurethane at −5 °C. After the mixture had been stirred for another 24 hours at ambient temperature, the yellow reaction mixture was poured into 50 g ice and stirred 1 hour. The white gum was collected and was dissolved in 300 mL ethyl acetate and washed five times (300 mL x 5) with water. The organic layer was dried with magnesium sulfate. After removal of the solvent in vacuo, the colorless oil was obtained.

– Synthesis of polynitramine

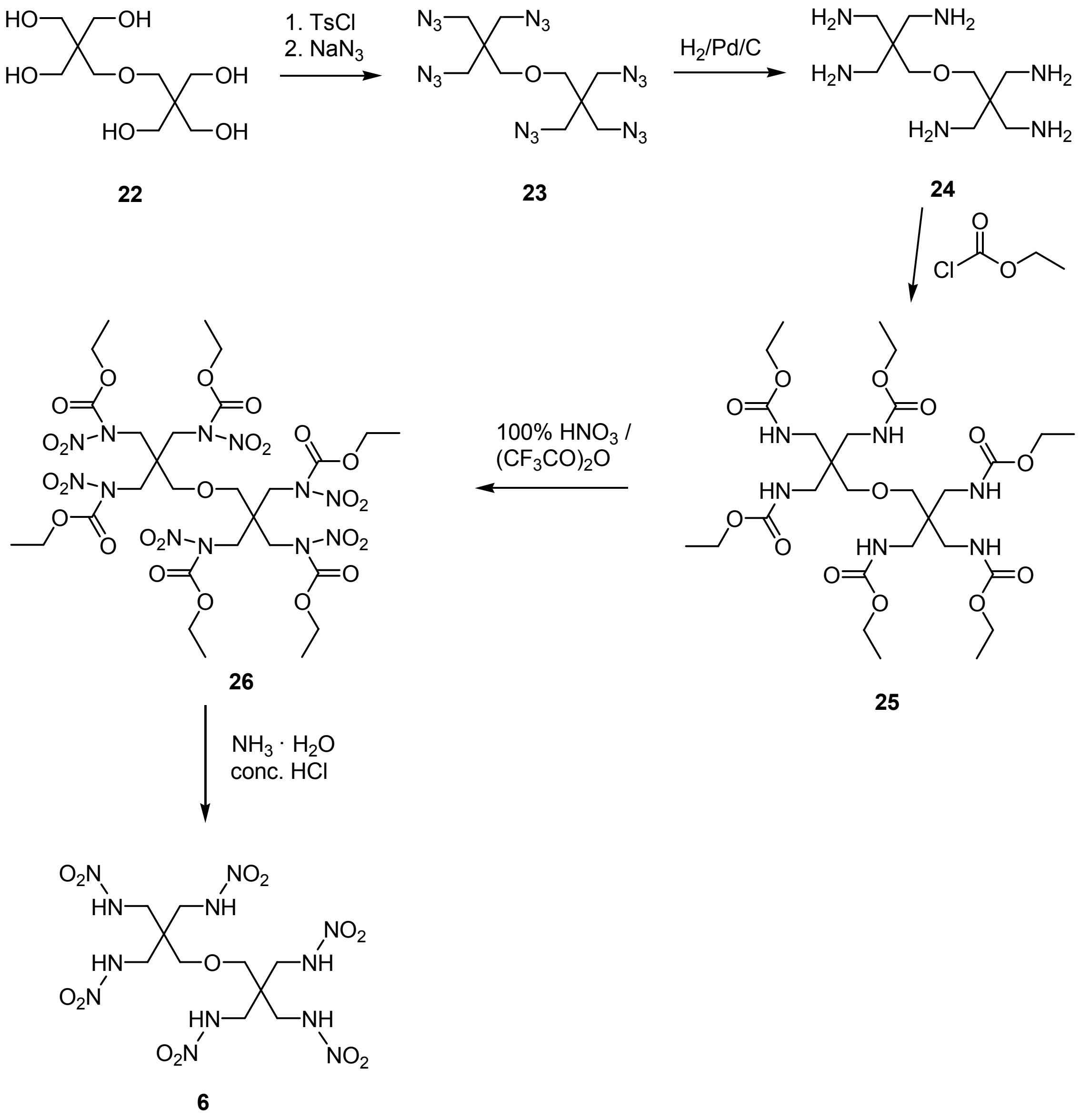
A solution of 5.0 mmol polynitrourethane in 50 mL ethanol and 150 mL of 28% aqueous ammonia was heated slowly at 50–60 °C (oil bath) for one hour (careful! ammonia fumes) and then refluxed at 90 °C (oil bath) for 18 hours (for compound **14**, 3 days are required). After cooling with ice, 36% hydrochloric acid was dropped into the reaction mixture until pH = 1. The aqueous layer was extracted three times with ethyl acetate (200 mL x 3). The combined organic extracts were washed five times (300 mL x 5) with water. The organic layer was dried with magnesium sulfate. After removal of the solvent in air, the white solid was obtained. The product was washed with acetonitrile.



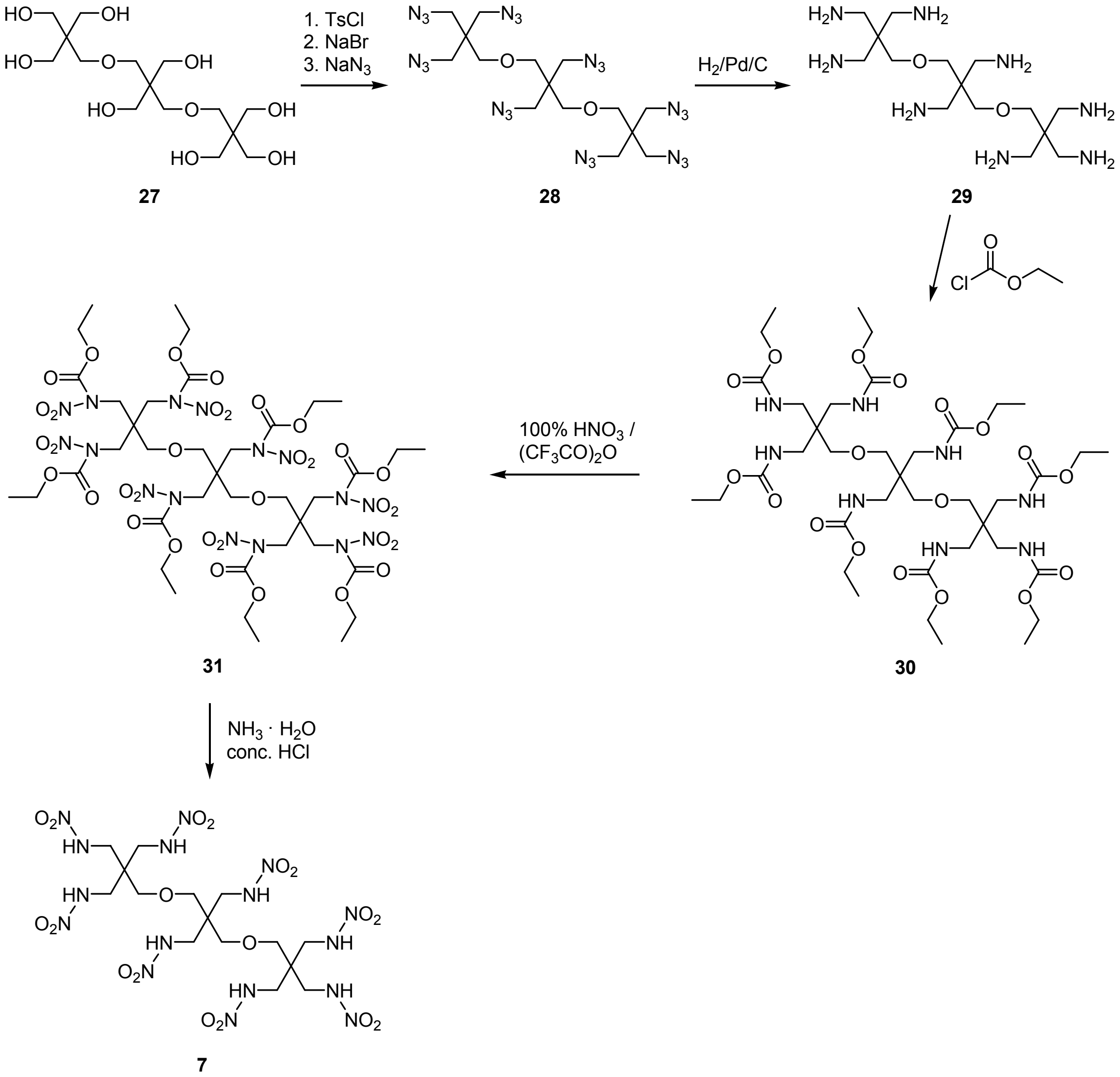
Scheme S1. Nitration of 1,2,3-triamino-2-(aminomethyl)propane (**11**); A: $H_2/Pd/C$, B: $ClCOOCH_2CH_3$, C: 100% $HNO_3/(CF_3CO)_2O$, D: 28% aq. NH_3/36% HCl.



Scheme S2. Synthesis of tris(nitramino)propane **5**.



Scheme S3. Synthesis of pentaerythrityl hexanitramine **6**.



Scheme S4. Synthesis of pentaerythrityl octanitramine **7**.

2: White solid; Yield 84%; M.p. 169 °C (dec.); IR (KBr): $\tilde{\nu}$ = 3389, 2983, 2936, 1699, 1518, 1308, 1243, 1159, 1130, 1027; ^{1}H NMR ([D$_6$]DMSO): δ = 1.16 (t, ^3J = 7.1 Hz, 12H, CH$_3$), 2.87, (d, ^3J = 6.5 Hz, 8H), 4.00 (q, ^3J = 7.1 Hz, 8H), 6.77 (t, ^3J = 6.4 Hz, 4H, NH); ^{13}C NMR ([D$_6$]DMSO): δ = 14.5, 41.5, 45.0, 60.1, 157.0; C,H,N analysis (%): calcd for $C_{17}H_{32}N_4O_8$ (420.46): C 48.56, H 7.67, N 13.33; found C 48.60, H 7.80, N 13.11.

3: Colorless oil; Yield 96%; IR (KBr): $\tilde{\nu}$ = 2988, 2940, 1771, 1590, 1294, 1236, 1178, 986, 858; ^{1}H NMR ([D$_6$]DMSO): δ = 1.29 (t, ^3J = 7.1 Hz, 12H, CH$_3$), 4.24 (s, 8H), 4.31 (q, ^3J = 7.1 Hz, 8H); ^{13}C NMR ([D$_6$]DMSO): δ = 13.5, 46.9, 51.1, 65.5, 151.6; ^{14}N NMR ([D$_6$]DMSO): δ = −36.5 (NO$_2$);^{15}N NMR ([D$_6$]DMSO): δ = −173.0, −36.8 (t, ^3J = 3.1 Hz, NO$_2$); C,H,N analysis (%): calcd for $C_5H_{12}N_8O_8$ (312.20): C 34.00, H 4.70, N 18.66; found C 34.42, H 4.71, N 16.80.

4: Colorless crystal; Yield 64%; M.p. 183 °C (dec.); IR (KBr): $\tilde{\nu}$ = 3356, 2995, 2963, 1545, 1446, 1411, 1343, 1281, 1153, 1099, 861, 543; ^{1}H NMR ([D$_6$]DMSO): δ = 3.63 (s, 8H, CH$_2$), 12.02 (s, 4H, NH); ^{13}C NMR ([D$_6$]DMSO): δ = 42.2, 46.4; ^{15}N NMR ([D$_6$]DMSO): δ = −207.6, −23.1 (NO$_2$); C,H,N analysis (%): calcd for $C_5H_{12}N_8O_8$ (312.20): C 19.24, H 3.87, N 35.89; found C 19.36, H 3.82, N 35.74.

5: White crystal; Yield 77%; M.p. 133 °C, 183 °C (dec.); IR (KBr): $\tilde{\nu}$ = 3370, 3283, 2958, 1589, 1431, 1346, 1271, 1148, 1125, 752; ^{1}H NMR ([D$_6$]DMSO): δ = 3.49 (dd, ^2J = 14.7 Hz, ^3J = 8.3 Hz, 2H), 3.74 (dd, ^2J = 14.7, ^3J = 4.5 Hz, 2H), 4.47 (m, 1H), 12.20 (s, 3H, NH); ^{3}C NMR ([D$_6$]DMSO): δ = 44.4, 51.4; ^{15}N NMR ([D$_6$]DMSO): δ = −202.1, −195.7, −19.6 (NO$_2$), −18.5 (NO$_2$); C,H,N analysis (%): calcd for $C_3H_8N_6O_6$ (224.13): C 16.08, H 3.60, N 37.50; found C 16.59, H 3.60, N 37.09.

6: White crystal; Yield 79%; Density = 1.607 g cm^{-3}; M.p. 181 °C (dec.); IR (KBr): $\tilde{\nu}$ = 3274, 3159, 2955, 2896, 1589, 1445, 1408, 1384, 1317, 1104; ^{1}H NMR ([D$_6$]DMSO): δ = 3.27 (s, 4H, CH$_2$), 3.60 (s, 12H, CH$_2$), 11.80 (br. s, 6H, NH); ^{3}C NMR ([D$_6$]DMSO): δ = 44.01, 46.12, 70.48; ^{15}N NMR ([D$_6$]DMSO): δ = −202.3, −18.0 (NO$_2$); C,H,N analysis (%): calcd for $C_{10}H_{22}N_{12}O_{13}$ (518.35): C 23.17, H 4.28, N 32.43; found C 23.83, H 4.24, N 31.16.

7: White solid; Yield 90%; Density = 1.638 g cm^{-3}; M.p. 185 °C (dec.); IR (KBr): $\tilde{\nu}$ = 3358, 3145, 2951, 2890, 1584, 1447, 1410, 1380, 1337, 1157, 1092; ^{1}H NMR ($[D_6]$DMSO): δ = 3.26 (s, 4H), 3.60 (s, 16H), 11.94 (br. s, 8H, NH); ^{3}C NMR ($[D_6]$DMSO): δ = 43.7, 44.9, 45.7, 46.0, 70.5; ^{15}N NMR ($[D_6]$DMSO): δ = −202.1, −201.9, −18.0 (NO_2), −17.8 (NO_2); C,H,N analysis (%): calcd for $C_{15}H_{32}N_{16}O_{18}$ (724.51): C 24.87, H 4.45, N 30.93; found C 24.67, H 4.48, N 30.80.

11: Extremely hygroscopic colorless liquid; Yield 99%; IR (KBr): $\tilde{\nu}$ = 3333, 2920, 2637, 1575, 1475, 1385, 1322; ^{1}H NMR ($CDCl_3$): δ = 1.18 (s, 8H, NH_2), 2.56 (s, 6H, CH_2); ^{15}N NMR ($CDCl_3$): δ = −362.7, −342.2.

12: White solid; Yield 70%; M.p. 145 °C; IR (KBr): $\tilde{\nu}$ = 3337, 2985, 2934, 1699, 1528, 1263; ^{1}H NMR ($[D_6]$DMSO): δ = 1.16 (t, ^{3}J = 7.0 Hz, 12H, CH_3), 3.20 (d, ^{3}J = 5.7 Hz, 6H, CH_2), 3.93 (q, ^{3}J = 7.0 Hz, 2H, CH_2), 3.99 (q, ^{3}J = 7.0 Hz, 6H, CH_2), 6.39 (s, 1H, NH), 6.93 (t, ^{3}J = 6.0 Hz, 3H, NH); ^{13}C NMR ($[D_6]$DMSO): δ = 14.5, 14.6, 41.4, 59.5, 60.1, 60.2, 154.6, 157.1; C,H,N analysis (%): calcd for $C_{16}H_{30}N_4O_8$ (406.43): C 47.28, H 7.44, N 13.79; found C 47.42, H 7.50, N 13.51.

13: Colorless oil; Yield 96%; ^{1}H NMR ($[D_6]$DMSO): δ = 1.13 (t, ^{3}J = 7.1 Hz, 3H, CH_3), 1.28 (t, ^{3}J = 7.1 Hz, 9H, CH_3), 3.93 (q, ^{3}J = 7.1 Hz, 2H, CH_2), 4.29 (q, ^{3}J = 7.1 Hz, 6H, CH_2), 4.51 (s, 6H, CH_2), 6.74 (s, 1H, NH); ^{13}C NMR ($[D_6]$DMSO): δ = 13.6, 14.4, 51.7, 59.7, 60.3, 65.3, 151.4, 155.0; ^{15}N NMR ($[D_6]$DMSO): δ = −284.7 (d, ^{1}J = 93 Hz), −169.7, −33.2 (NO_2); C,H,N analysis (%): calcd for $C_{16}H_{26}N_7O_{14}\cdot H_2O$ (559.44): C 34.35, H 5.22, N 17.53; found C 34.50, H 4.79, N 16.73.

14: light brown gum; Yield 75%; M.p. 157−180 °C (dec.); IR (KBr): $\tilde{\nu}$ = 3377, 2985, 1703, 1585, 1528, 1412, 1382, 1318, 1255, 1080, 565; ^{1}H NMR ($[D_6]$DMSO): δ = 1.17 (t, ^{3}J = 7.1 Hz, 3H, CH_3), 3.85 (s, 6H, CH_2), 3.97 (q, ^{3}J = 7.1 Hz, 2H, CH_2), 7.18 (s, 1H, NH), 12.10 (s, 3H, NH); ^{13}C NMR ($[D_6]$DMSO): δ = 14.5, 46.1, 57.0, 59.8, 154.9; ^{15}N

NMR ([D$_6$]DMSO): δ = −286.2, −202.8, −18.5 (NO$_2$); C,H,N analysis (%): calcd for $C_7H_{15}N_7O_8 \cdot 1/4C_4H_8O_2$ (ethyl acetate) (325.24): C 27.67, H 4.93, N 28.23; found C 27.94, H 5.06, N 28.94.

15$\cdot H_2O$**:** White solid; Yield 83%; M.p. 138 °C, 197−205°C (dec.); IR (KBr): $\tilde{\nu}$ = 3415, 3336, 3269, 3202, 3063, 2981, 2713, 2629, 1705, 1613, 1547, 1449, 1418, 1340, 1281, 1262, 1078, 946; ^{1}H NMR ([D$_6$]DMSO): δ = 1.11 (t, ^3J = 7.1 Hz, 3H, CH$_3$), 3.46 (s, 6H), 3.87 (q, ^3J = 7.1 Hz, 2H), 6.41 (s, 1H, NH), 6.77 (br. s, 15H); ^{13}C NMR ([D$_6$]DMSO): δ = 14.7, 54.0, 56.4, 59.2, 154.6; ^{15}N NMR ([D$_6$]DMSO): δ = −323.9, −282.8 (d, ^1J = 89 Hz), −131.8, −14.7 (NO$_2$); C,H,N analysis (%): calcd for $C_{17}H_{27}N_{13}O_8 \cdot H_2O$ (439.39): C 19.13, H 6.65, N 41.44; found C 19.24, H 6.61, N 41.88.

19: Extremely hygroscopic colorless liquid; Yield 73% (from tosylate **15**); IR (KBr): $\tilde{\nu}$ = 3352, 1576, 1482, 1385, 1324; ^{1}H NMR (CDCl$_3$): δ = 1.49 (br. s, 6H, NH$_2$), 2.38−2.44 (m, 2H, CH$_2$), 2.52−2.61 (m, 1H, CH), 2.62−2.68 (m, 2H, CH$_2$); ^{13}C NMR ([D$_6$]DMSO): δ = 46.3, 55.7.

20: White solid; Yield 34%; M.p. 110 °C; IR (KBr): $\tilde{\nu}$ = 3322, 2983, 2939, 1686, 1545, 1288, 1261, 1156, 1071, 1034; ^{1}H NMR ([D$_6$]DMSO): δ = 1.14 (t, ^3J = 7.1 Hz, 9H, CH$_3$), 2.93−3.10 (m, 4H), 3.54 (sext, ^3J = 6.5 Hz, 1H), 3.95 (q, ^3J = 7.1 Hz, 2H), 3.96 (q, ^3J = 7.1 Hz, 4H), 6.75 (d, ^3J = 8.2 Hz, 1H, NH), 6.96 (t, ^3J = 4.7 Hz, 2H, NH); ^{13}C NMR ([D$_6$]DMSO): δ = 14.57, 14.61, 41.7, 51.0, 59.2, 59.7, 155.9, 156.5; C,H,N analysis (%): calcd for $C_{12}H_{23}N_3O_6$ (305.33): C 47.20, H 7.59, N 13.76; found C 47.25, H 7.75, N 14.32.

21: Colorless oil; Yield 97%; ^{1}H NMR ([D$_6$]DMSO): δ = 1.23 (t, ^3J = 6.9 Hz, 3H) , 1.26 (t, ^3J = 7.1 Hz, 6H), 4.24−4.34 (m, 6H), 4.47 (dd, ^2J = 16.2 Hz, ^3J = 4.0 Hz, 2H), 4.74 (dd, ^2J = 16.2 Hz, ^3J = 9.0 Hz, 2H), 5.16 (m, 1H); ^{13}C NMR ([D$_6$]DMSO): δ = 13.5, 13.5, 47.9, 57.4, 65.0, 65.4, 149.3, 149.6; ^{15}N NMR ([D$_6$]DMSO): δ = −169.9, −167.8, −36.0 (NO$_2$), −35.4 (NO$_2$); C,H,N analysis (%): calcd for $C_{12}H_{20}N_6O_{12}$ (440.32): C 32.73, H 4.58, N 19.09; found C 32.71, H 4.58, N 19.57.

24: Extremely hygroscopic colorless liquid; Yield 96%; IR (KBr): $\tilde{\nu}$ = 3295, 3081, 2932, 1642, 1549, 1436, 1386, 1294; ^{1}H NMR ($CDCl_3$): δ = 1.11 (s, 12H, NH_2), 2.61 (s, 12H), 3.25 (s, 4H); ^{13}C NMR ($CDCl_3$): δ = 43.2, 43.7, 73.3.

25: White solid; Yield 73%; M.p. 265 °C; IR (KBr): $\tilde{\nu}$ = 3331, 2981, 2939, 2874, 1699, 1527, 1302, 1253, 1134, 1029; ^{1}H NMR ([D_6]DMSO): δ = 1.16 (br. s, 18H), 2.93 (s, 4H), 3.34 (br. s, 12H), 4.00 (br. s, 12H), 6.88 (br. s, 6H, NH); ^{13}C NMR ([D_6]DMSO): δ = 14.6, 41.0, 44.9, 60.2, 70.1, 157.1; C,H,N analysis (%): calcd for $C_{28}H_{52}N_6O_{13}$ (680.74): C 49.40, H 7.70, N 12.35; found C 49.41, H 7.71, N 12.23.

26: Colorless oil; Yield 95%; ^{1}H NMR ([D_6]DMSO): δ = 1.28 (t, ^3J = 7.1 Hz, 18H, CH_3), 3.25 (s, 4H, CH_2), 4.24 (s, 12H, CH_2), 4.30 (q, ^3J = 7.1 Hz, 12H, CH_2); ^{13}C NMR ([D_6]DMSO): δ = 13.6, 46.3, 50.4, 65.3, 72.0, 151.3; ^{15}N NMR ([D_6]DMSO): δ = −169.1, −32.2 (NO_2); C,H,N analysis (%): calcd for $C_{28}H_{46}N_{12}O_{25}$ (950.73): C 35.37, H 4.88, N 17.68; found C 35.14, H 4.79, N 16.74.

29: Extremely hygroscopic colorless liquid; Yield 99%; ^{1}H NMR ([D_6]DMSO): δ = 1.92 (br. s, 16H, NH_2), 2.40 (s, 12H), 2.43 (s, 4H), 3.13 (s, 4H), 3.16 (s, 4H); ^{13}C NMR ([D_6]DMSO): δ = 42.8, 43.7, 44.3, 71.7, 72.7; ^{1}H NMR ($CDCl_3$): δ = 1.67 (s, 16H, NH_2), 2.39 (s, 16H), 3.13 (s, 4H), 3.16 (s, 4H); ^{15}N NMR ($CDCl_3$): δ = −361.7 (s, NH_2).

30: White solid; Yield 81%; M.p. 266 °C; IR (KBr): $\tilde{\nu}$ = 3331, 3073, 2980, 2938, 2875, 1699, 1523, 1302, 1253, 1134, 1028; ^{1}H NMR ([D_6]DMSO): δ = 1.16 (s, 24H), 2.93 (s, 16H), 3.34 (s, 8H), 4.00 (s, 16H), 6.88 (s, 8H, NH); ^{13}C NMR ([D_6]DMSO): δ = 14.6 (8C), 41.0 (8C), 44.9 (2C), 60.2 (8C), 70.1 (4C), 157.1 (8C); C,H,N analysis (%): calcd for $C_{39}H_{72}N_8O_{18}$ (941.03): C 49.78, H 7.71, N 11.91; found C 49.99, H 7.82, N 12.26.

31: Colorless oil; Yield 92%; ^{1}H NMR ([D_6]DMSO): δ = 1.29 (t, ^3J = 7.1 Hz, 24H), 3.23 (s, 4H), 3.28 (s, 4H), 4.20 (s, 4H), 4.26 (s, 12H), 4.34 (q, ^3J = 7.1 Hz, 16H); ^{13}C NMR ([D_6]DMSO): δ = 13.5 (8C), 45.5, 46.3, 50.6, 50.8, 65.1, 65.2, 71.3, 71.9, 151.2, 151.3; C,H,N analysis (%): calcd for $C_{39}H_{64}N_{16}O_{34}$ (1301.01): C 36.00, H 4.96, N 17.23; found C 35.94, H 5.01, N 16.95.

^{1}H, ^{13}C, ^{14}N and ^{15}N NMR spectra

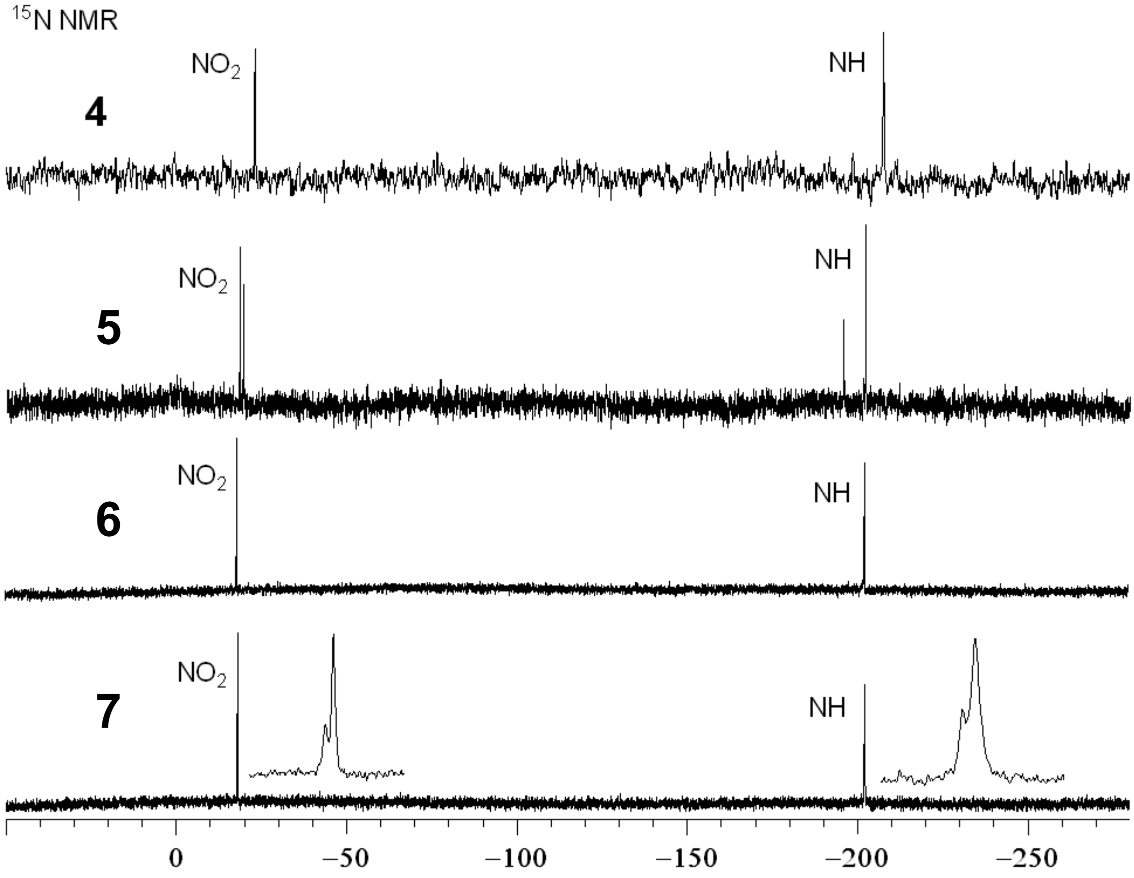


Figure S1. ^{15}N NMR spectra of **4**−**7** in [D$_6$]DMSO.

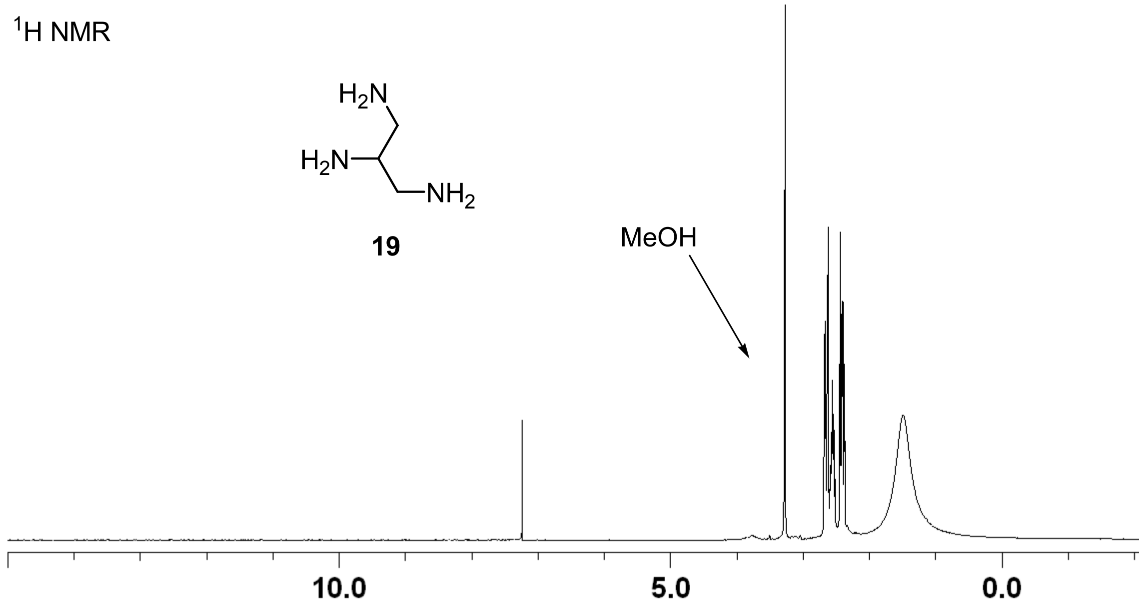


Figure S2.

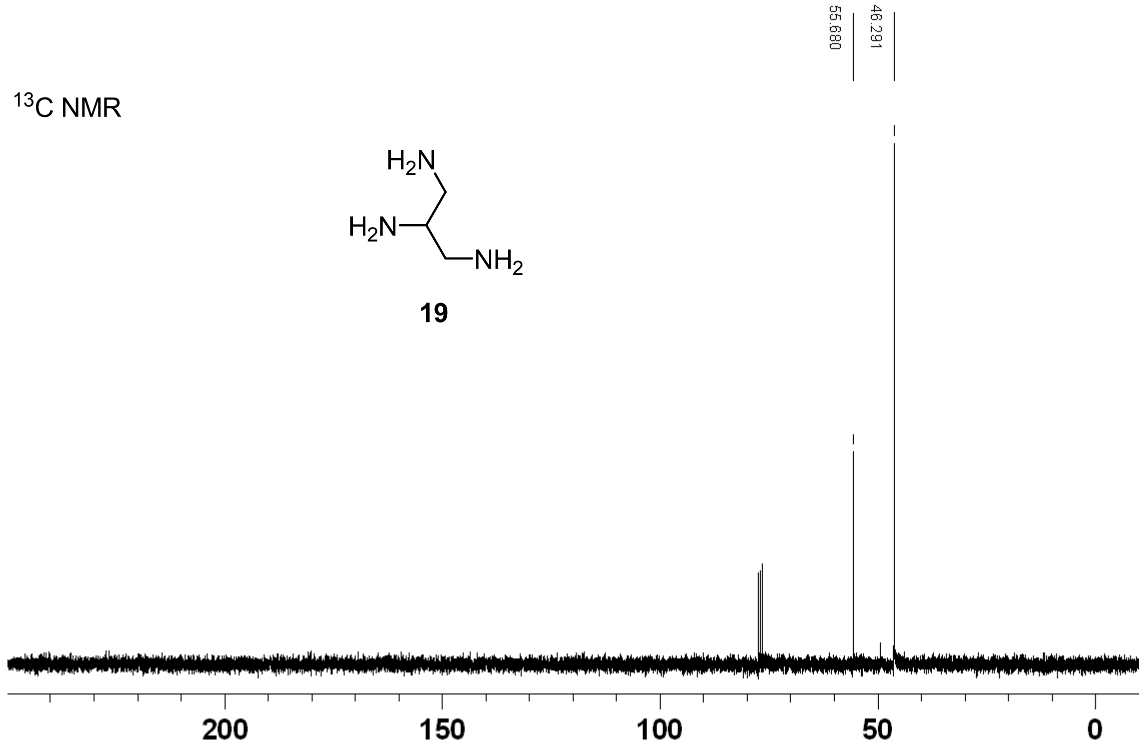


Figure S3.

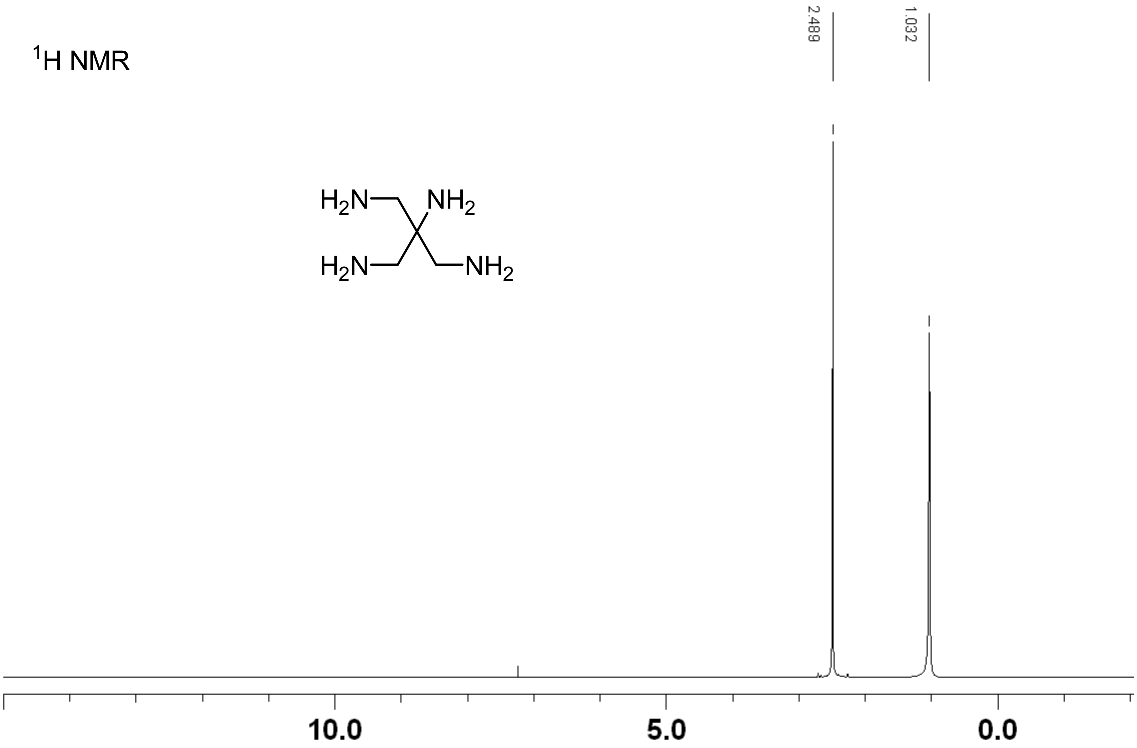


Figure S4.

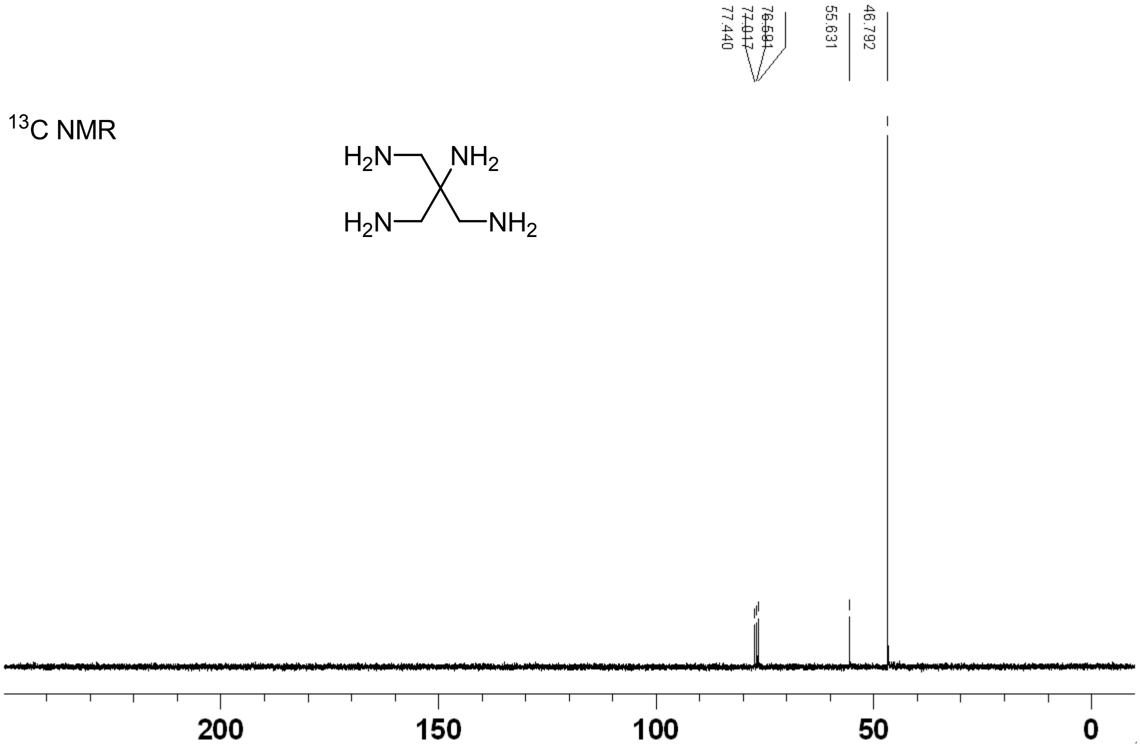


Figure S5.

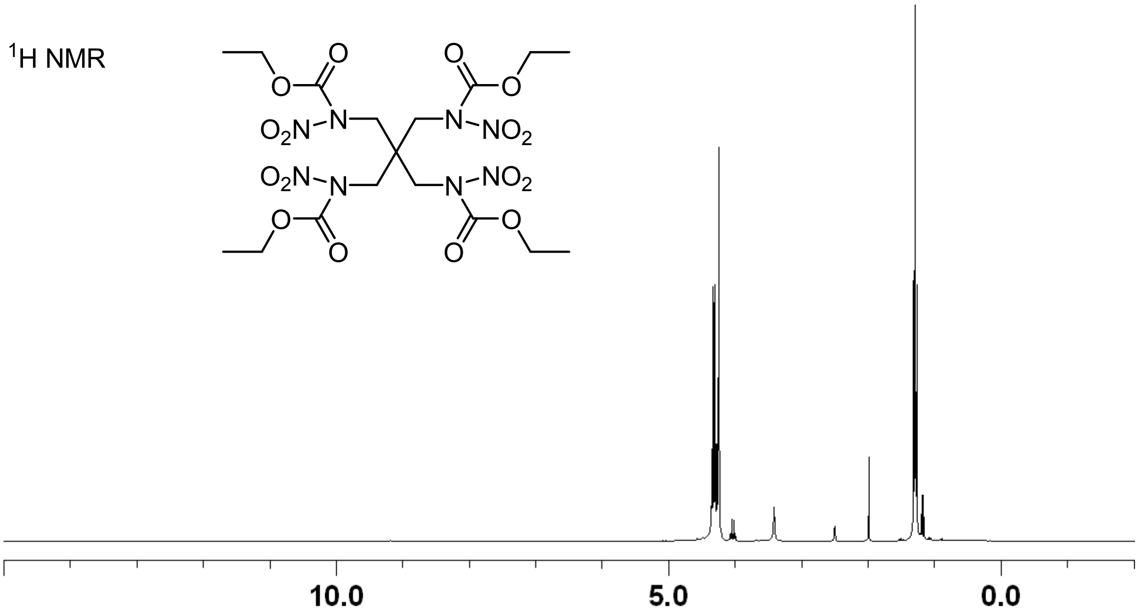


Figure S6.

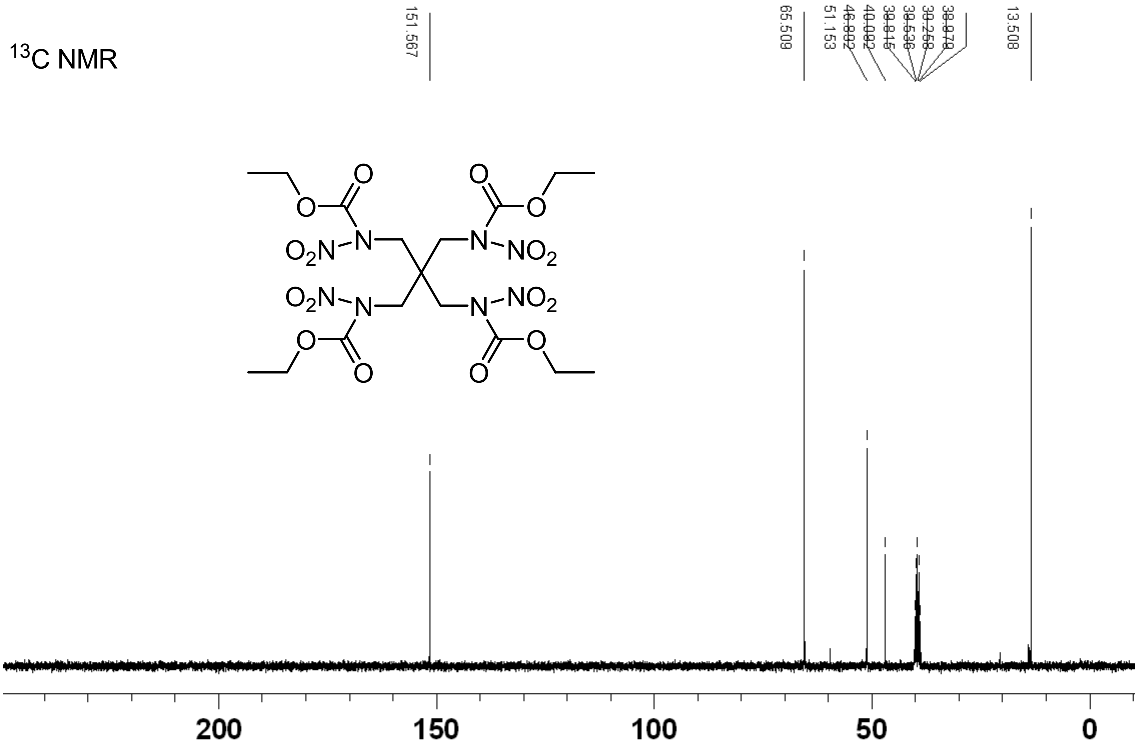


Figure S7.

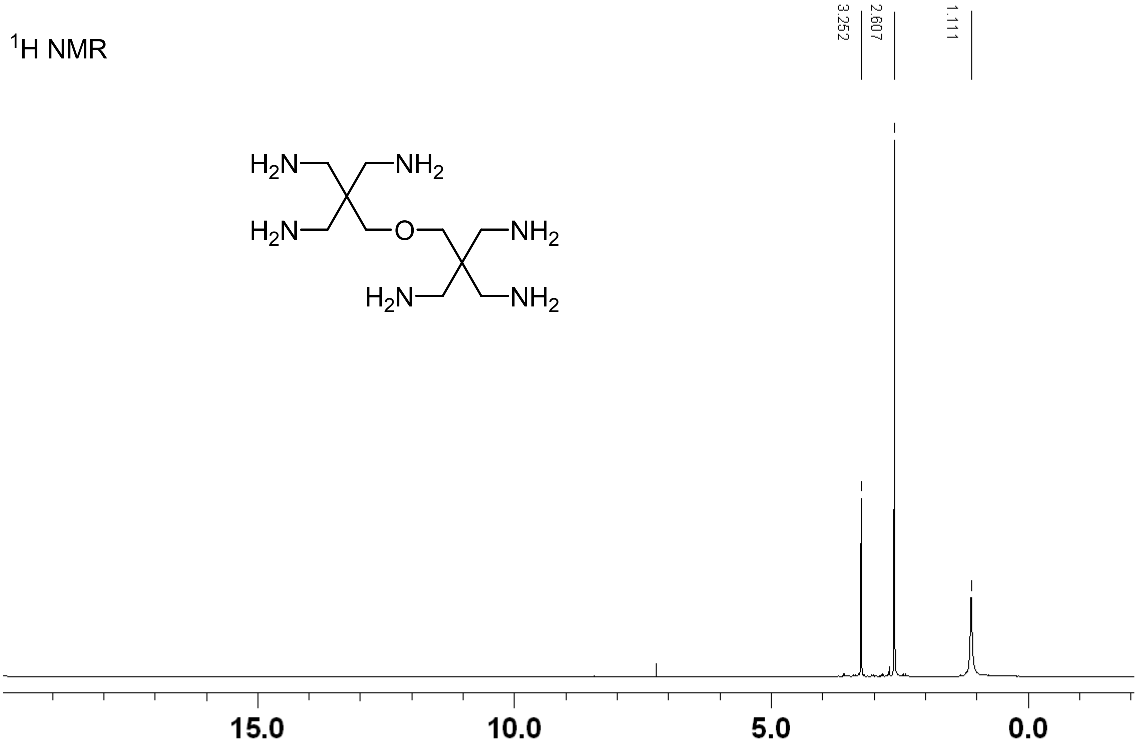


Figure S8.

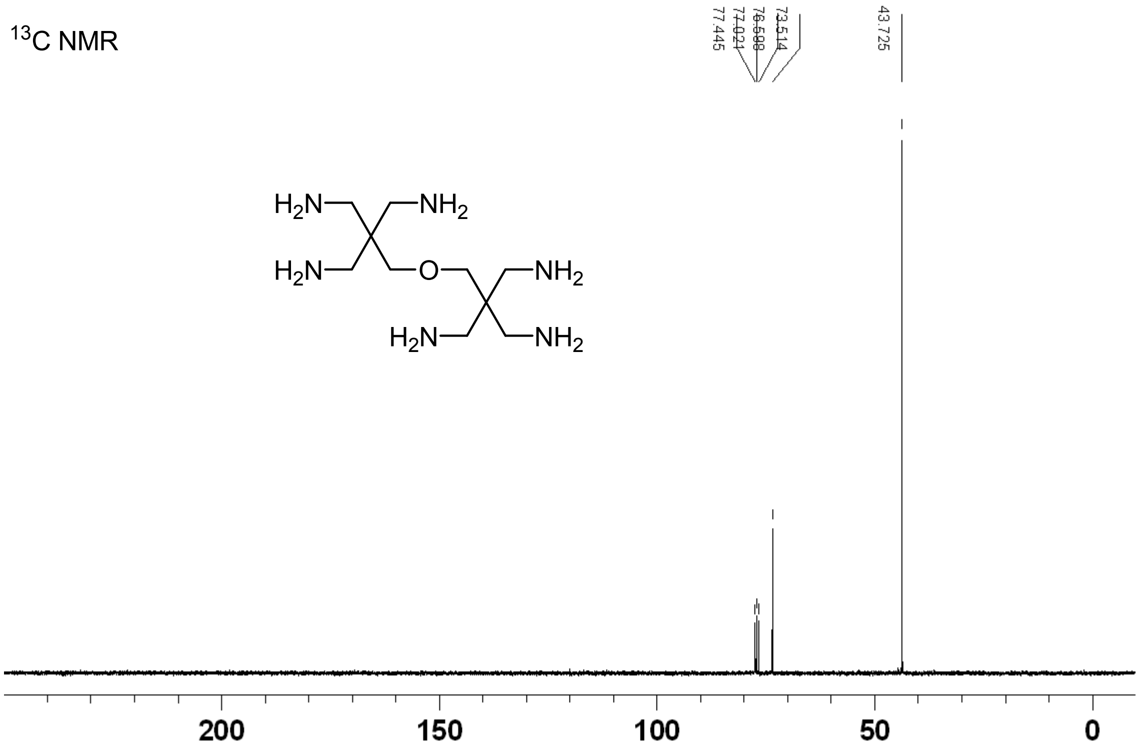


Figure S9.

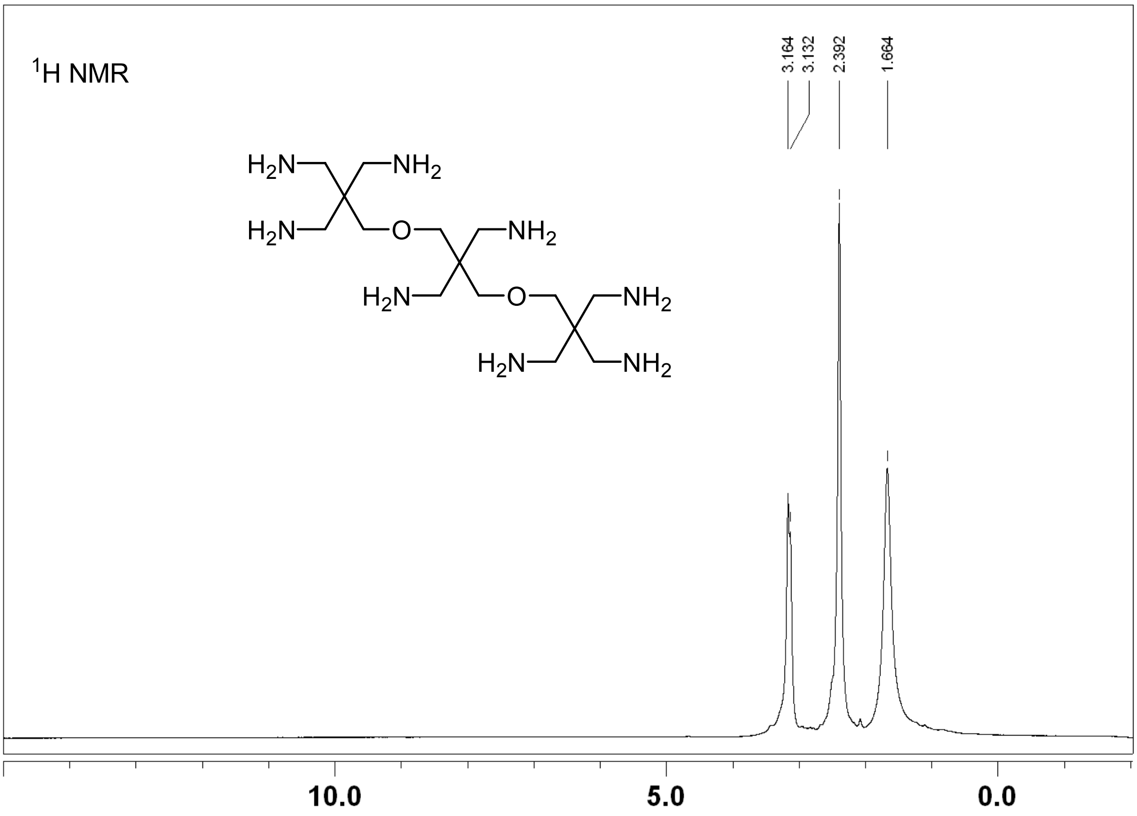


Figure S10.

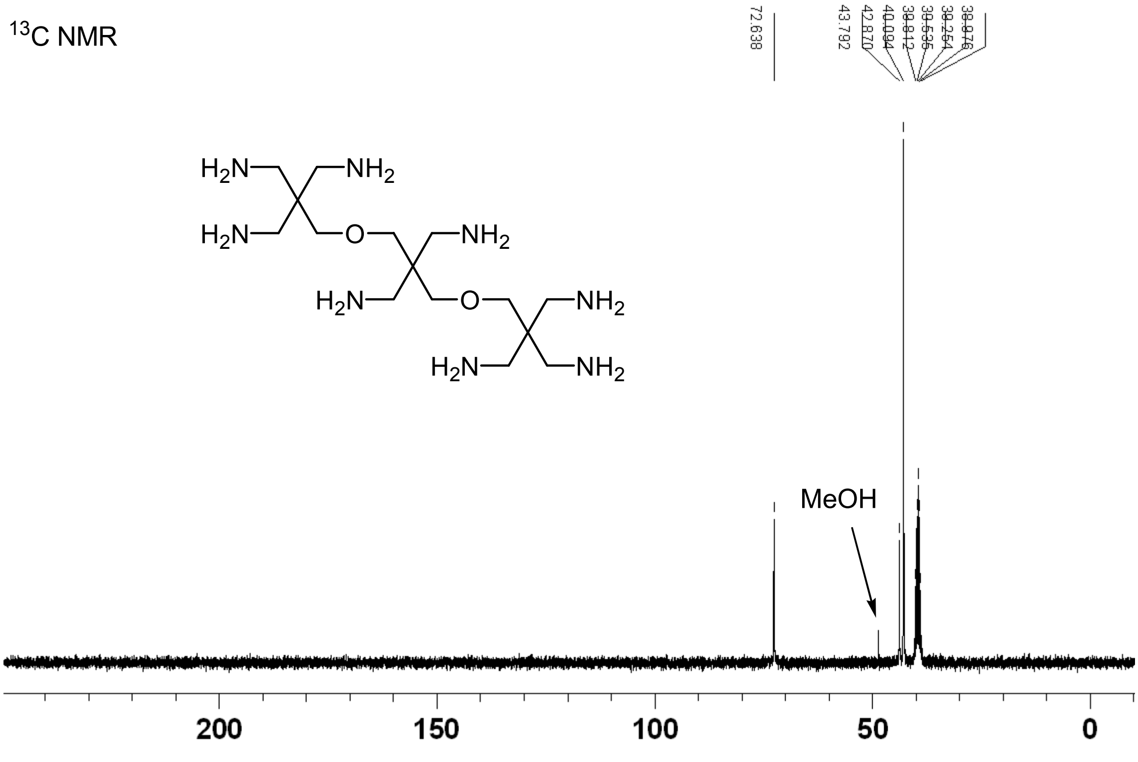


Figure S11.

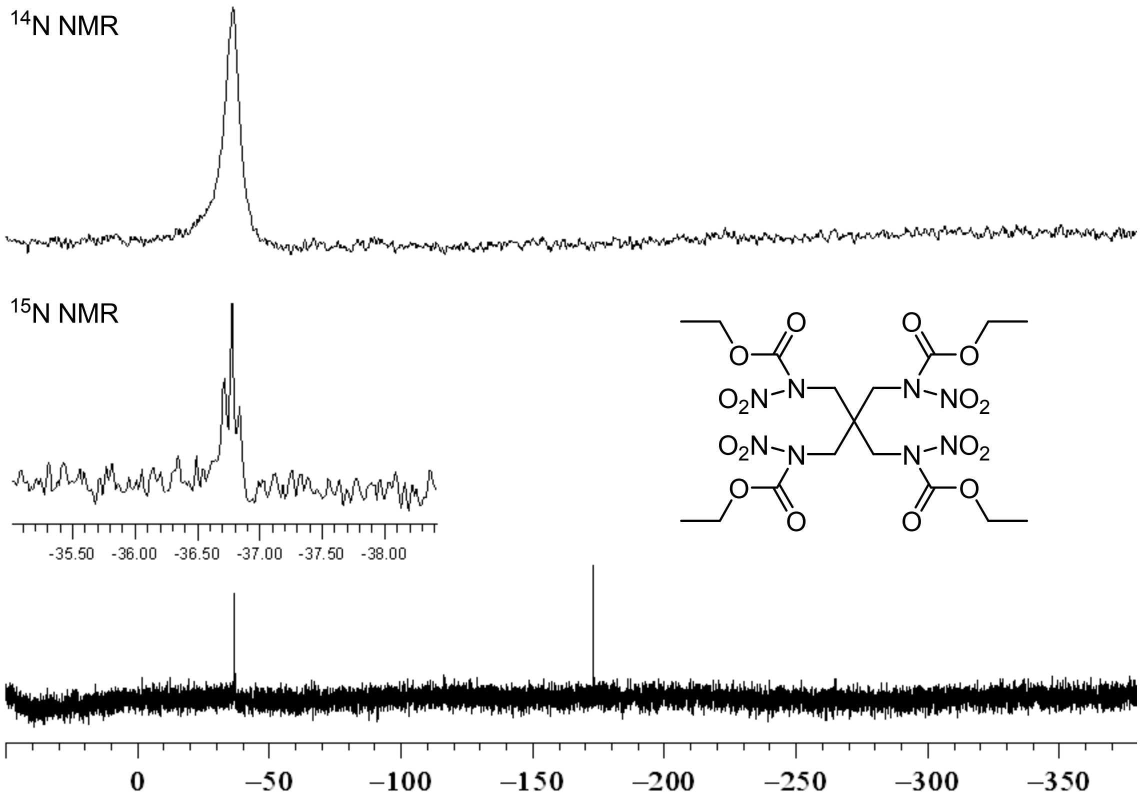


Figure S12.

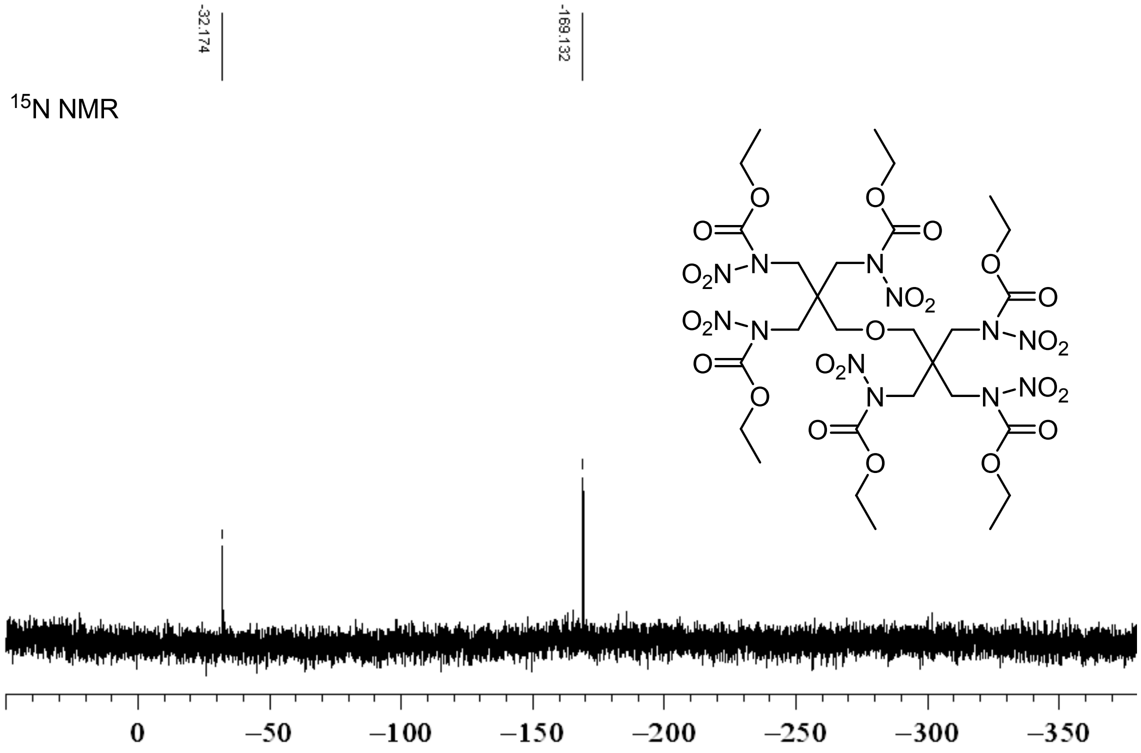


Figure S13.

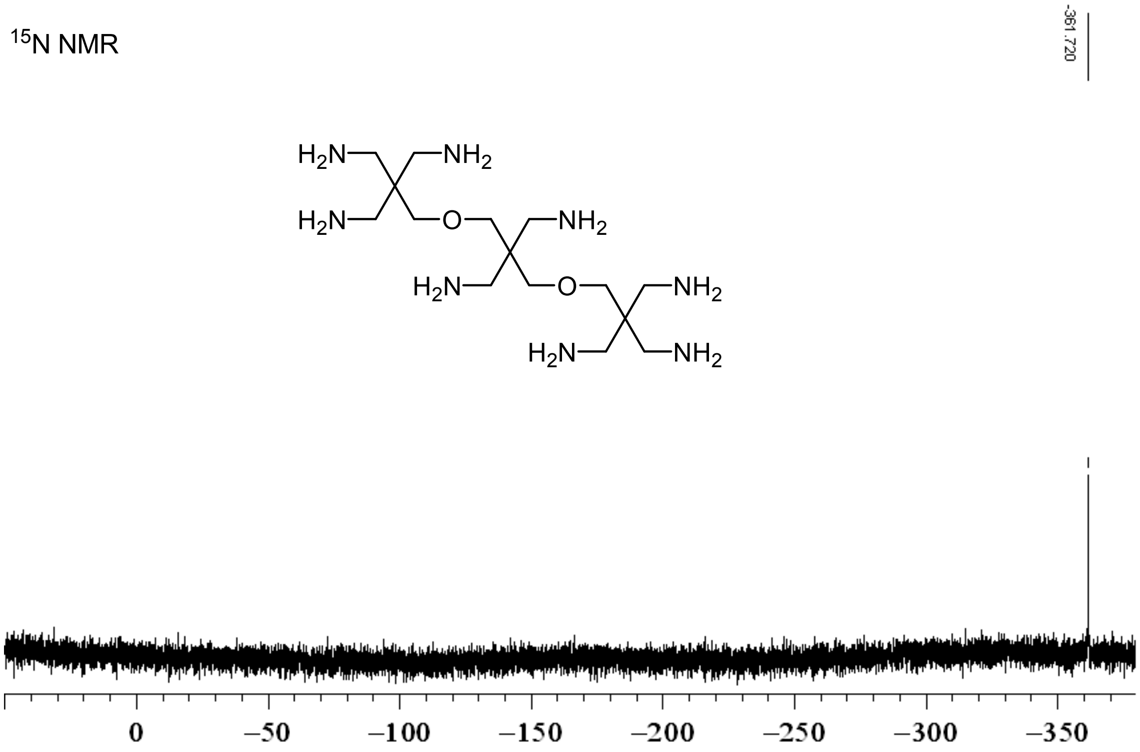


Figure S14.

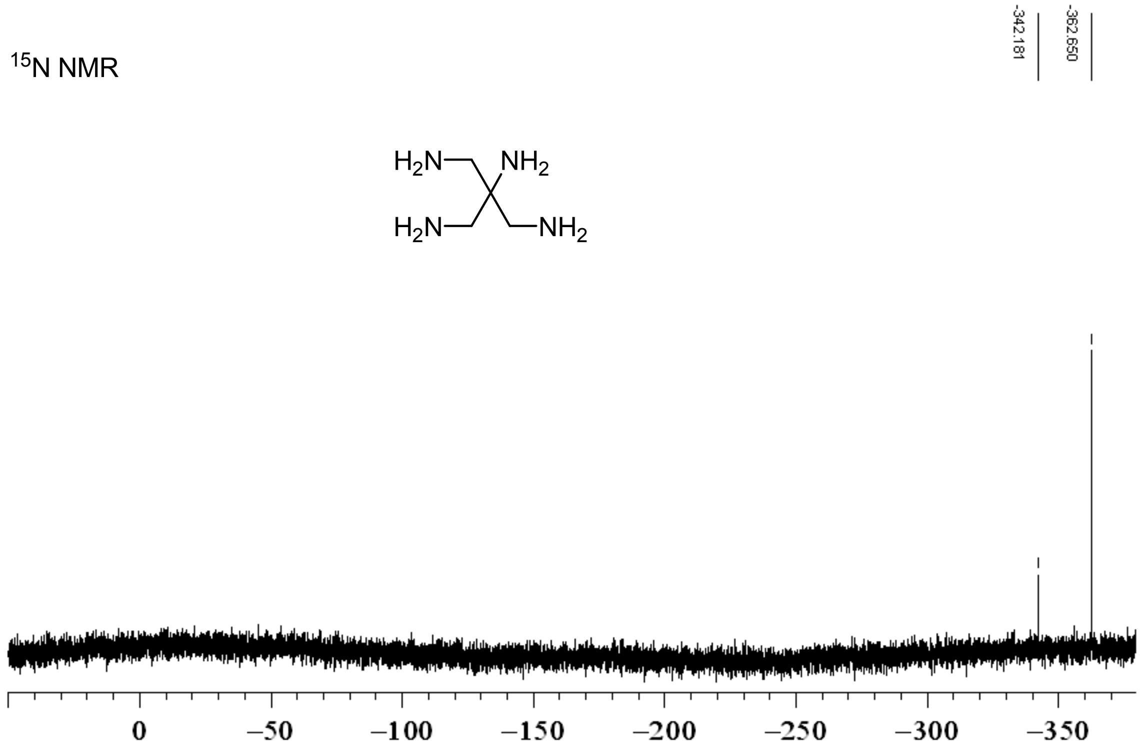


Figure S15.

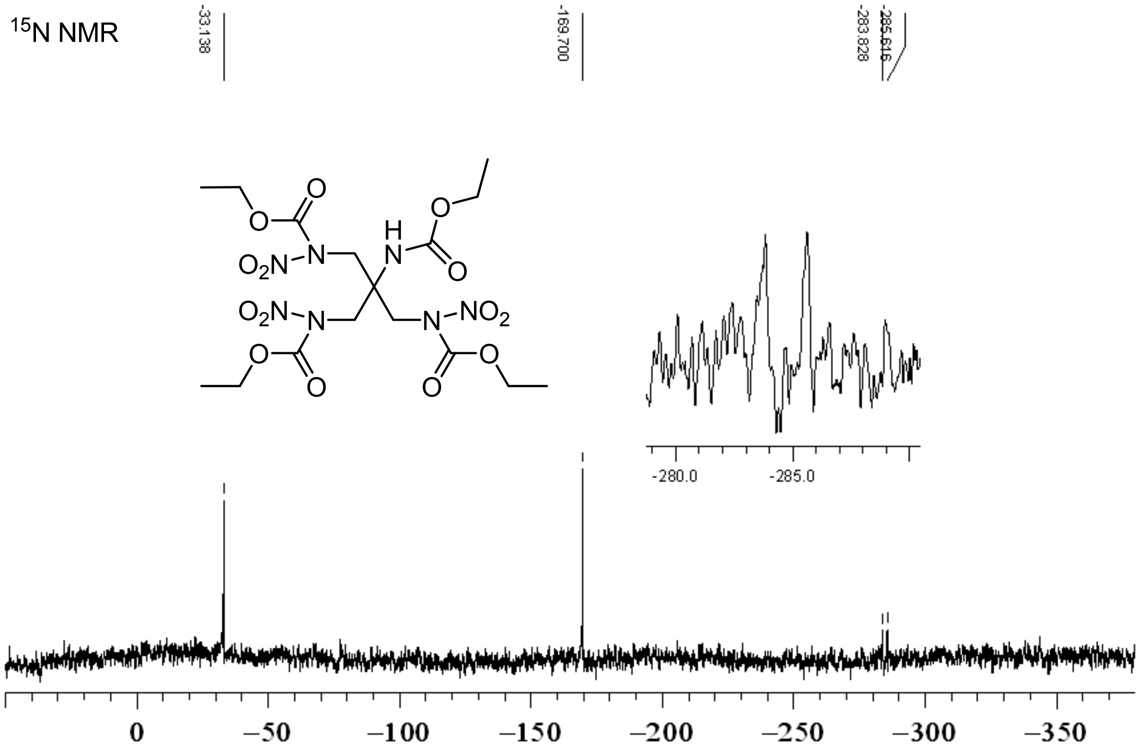


Figure S16.

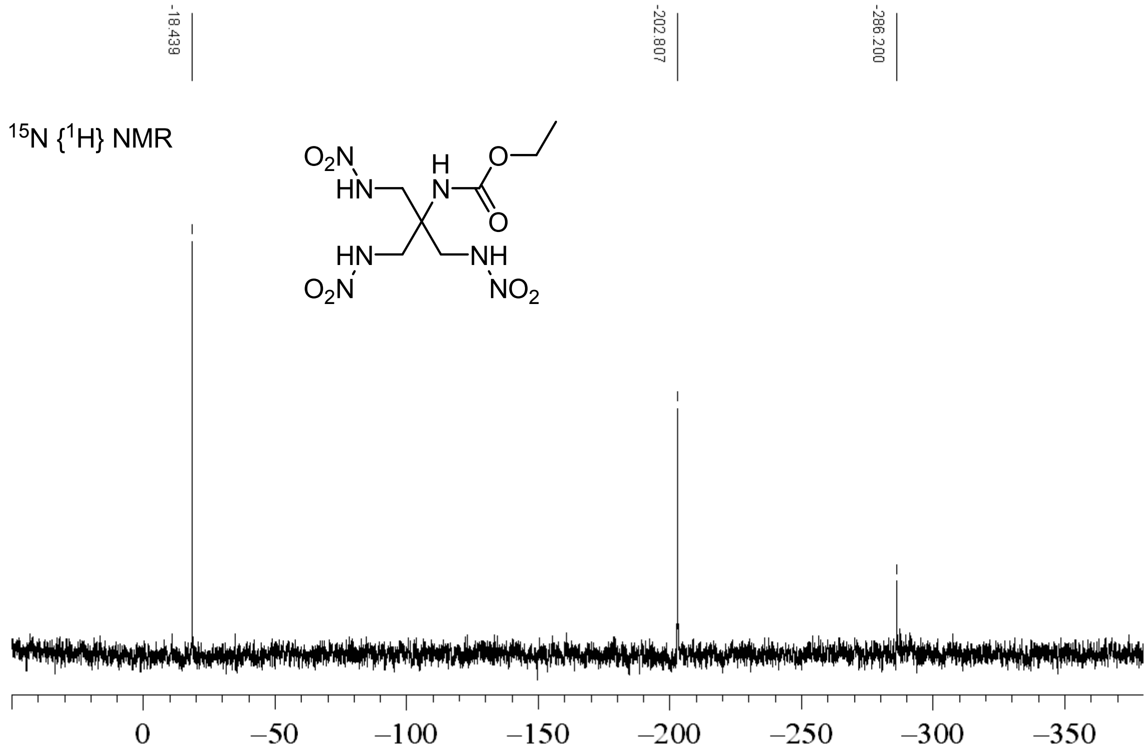


Figure S17.

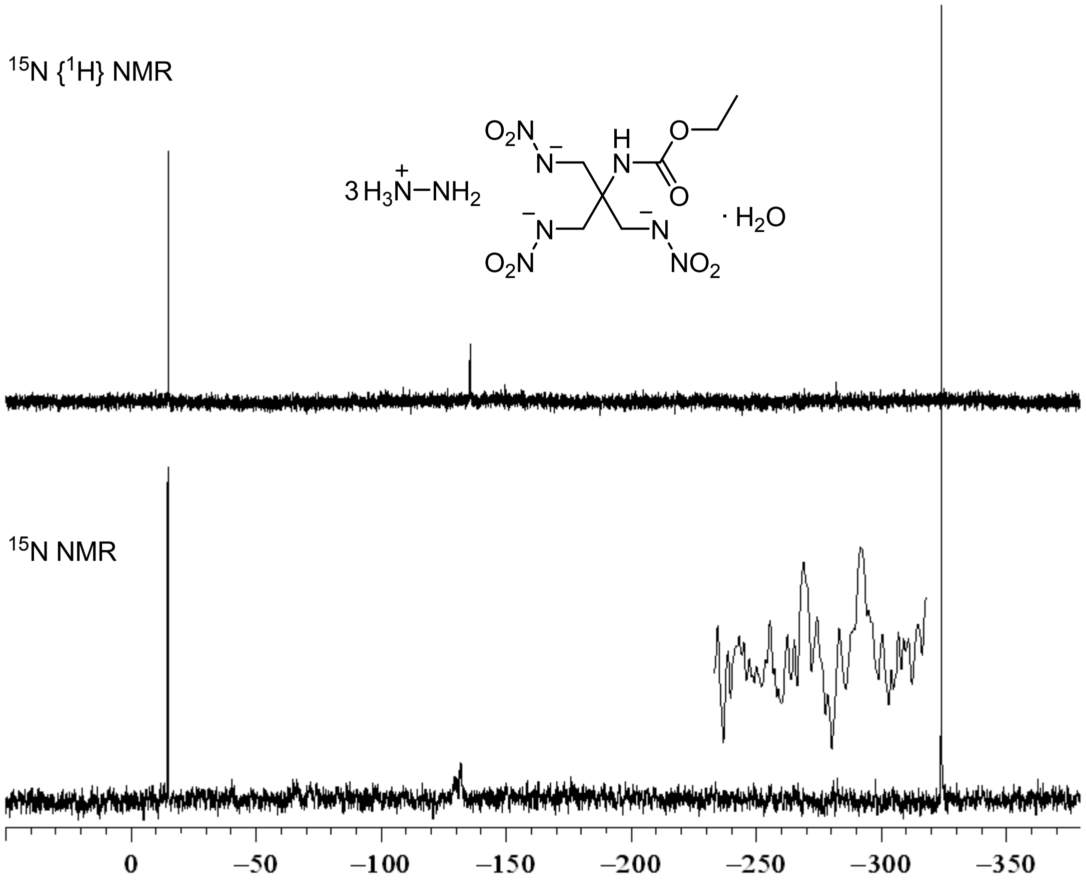


Figure S18.

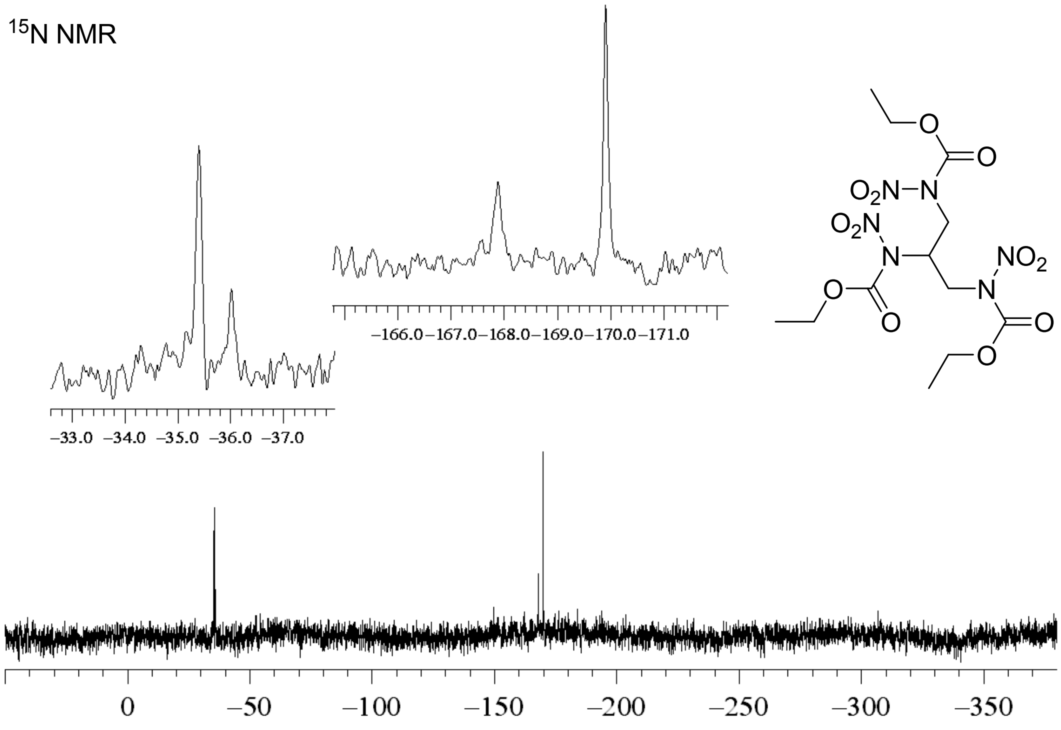
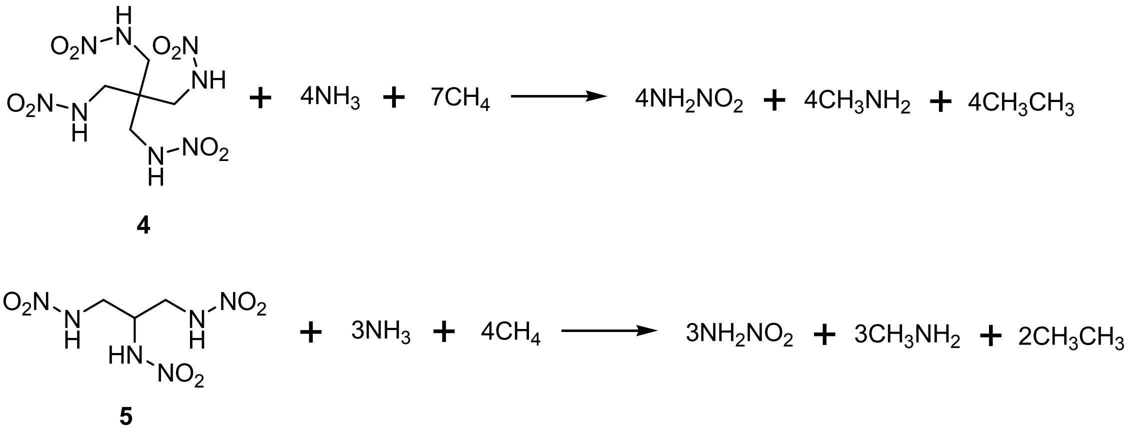


Figure S19.

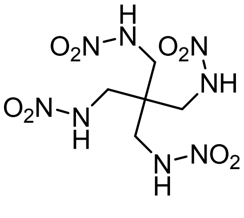
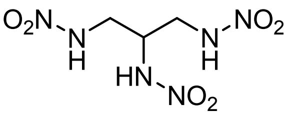
Computational data

The remaining task is to determine the heats of formation of the polynitramines **4** and **5**; these values were computed by using the method of isodesmic reactions (Scheme S5). Calculations were carried out by using the Gaussian 03 (Revision D.01) suite of programs.[2] The geometric optimization of the structures and frequency analyses were carried out by using the B3LYP functional with the 6-31+G** basis set, and single-point energies were calculated at the MP2/6-311++G** level.



Scheme S5

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 (gaseous state) (HoF) [kJ/mol] of the compounds.

	E_0	ZPE	H_T	HoF
 **4**	−1234.394906	0.24192	0.02162	23.38801372 −60.3 (solid state)
 **5**	−896.5416121	0.162811	0.01157	408.6034117 324.9 (solid state)

References

1 (*a*) D. D. Diaz, S. Punna, P. Holzer A. K., McPherson, K. B. Sharpless, V. V. Fokin, and M. G. Finn, *J. Polym. Sci. Part A*, 2004, **42**, 4392. (*b*) Y.-H. Joo and J. M. Shreeve, *Inorg. Chem.*, 2009, ASAP. DOI: 10.1021/ic901019p. (*c*) A. Zimmer, I. Müller, G. J. Reiß, A. Caneschi, D. Gatteschi and K. Hegetschweiler, *Eur. J. Inong. Chem.*, 1998, 2079. (*d*) E. B. Fleischer, A. E. Gebala, A. Levey and P. A. Tasker, *J. Org. Chem.*, 1971, **36**, 3042. (*e*) W. S. Anderson and H. J. Hyer, *CPIA Publ.*, 1981, **340**, 387.

2 Gaussian 03 (Revision D.01): M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.