Supporting Information

Energetic Salts from Phenolate Derivatives

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Table 1. Total Energy (E_0), Zero Point Energy (ZPE) and Thermal Correction (ΔH_T) at the B3PW91/6-31G(d,p) Level, gas phase heat of formation, molecular surface properties, heat of sublimation and calculated solid state heat of formation for the heterocyclic compounds selected for salt preparation.

Compd.	E_0[a]	ZPE[b]	ΔH_T[c]	HOF_{Gas}[d]	A[e]	σ^2_{tot}[f]	ν[g]	HOF_{Sub}[h]	HOF_{Solid}[i]
4-Amino-4H-1,2,4-triazole	-297.36933	0.0764	0.0059	336.02	114.21	445.85	0.25	99.86	236.16
3-Amino-1,2,4-triazole	-297.42696	0.0763	0.0056	171.11	112.32	240.37	0.24	78.98	92.13 (77)[2]
3,5-Diamino-1,2,4-triazole	-352.75304	0.0942	0.0074	157.90	127.75	272.84	0.24	86.55	71.35
3,4-Diaminofurazan	-372.54123	0.0782	0.0069	196.34 (143)[1]	122.90	411.67	0.22	95.57	100.77
Guanidine	-205.22149	0.0766	0.0055	31.06	97.43	262.99	0.24	77.98	-46.92 (-56)[3]

[a]Total energy (a.u.). [b]Zero point energy (a.u.). [c]Thermal correction (a.u.). [d]Heat of formation in gas phase (kJ/mol). [e]Area of the isosurface of 0.001 electrons/bohr^3 electronic density (Å^2). [f]Measure of variability of the electrostatic potential (kJ/mol). [g]Degree of balance between the positive and negative surface potentials. [h]Heat of sublimation (kJ/mol). [i]Heat of formation in solid state (kJ/mol).

References:

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Table 2. Total Energy (E_0), Zero Point Energy (ZPE) and Thermal Correction (ΔH_T) at the B3PW91/6-31G(d,p) Level and gas phase heat of formation, molecular surface properties, heat of sublimation and calculated solid state heat of formation for the nitrophenols.

Compd.	E_0[a]	**ZPE**[b]	ΔH_T[c]	HOF_{Gas}[d]	**A**[e]	σ^2_{tot}[f]	ν[g]	HOF_{Sub}[h]
Picric acid	-920.49172	0.1131	0.0128	-172.12	205.52	132.38	0.21	96.32
2,4,6-Trinitro-m-cresol	-959.76295	0.1411	0.0154	-196.86	222.13	96.02	0.22	99.28
3-Azido-2,4,6-trinitrophenol	-1083.99084	0.1160	0.0166	135.46	235.68	138.71	0.18	109.20
Styphnic acid	-995.68373	0.1173	0.0135	-386.42	209.51	136.40	0.22	99.00
2,4,6-Trinitro-1,3,5-benzenetriol	-1070.87403	0.1219	0.0153	-549.57	216.67	161.04	0.20	104.50

[a]Total energy (a.u.). [b]Zero point energy (a.u.). [c]Thermal correction (a.u.). [d]Heat of formation in gas phase (kJ/mol). [e]Area of the isosurface of 0.001 electrons/bohr^3 electronic density (Å^2). [f]Measure of variability of the electrostatic potential (kJ/mol). [g]Degree of balance between the positive and negative surface potentials. [h]Heat of sublimation (kJ/mol).

Reported sensitivity studies of selective nitrophenols [R. Meyer, J. Kohler, A. Homburg, Explosives, 6th Ed., Wiley VCH, Weinheim, 2007]:

1. Picric acid:

Impact sensitivity: 0.75 kpm = 7.4 Nm

Friction sensitivity: up to 353 N

Critical diameter of steel sleeve test: 4 mm

2. Styphnic acid:

Impact sensitivity: 0.75 kp m = 7.4 N m

Friction sensitivity: at 36 kg = 353 N

Critical diameter of steel sleeve test: 14 mm

3. 2,4,6-Trinitrocresol:

Impact sensitivity: 1.2 kp m = 12 N m

Friction sensitivity: up to 36 kp = 353 N

Computational Details

The geometries of the designed compounds were fully optimized without any symmetry restriction using density functional theory (DFT) at the B3PW91 functional with the 6-31G(d,p) basis set in the Gaussian 03 software package.[1] All of the optimized structures were characterized to true local energy minima on the potential-energy surface without imaginary frequencies. The isodesmic reaction used for the prediction of gas phase HOF (HOF_{Gas}) of designed compounds is shown in Scheme 7. For estimation of the potential performance of the energetic material, it is also significant to calculate their solid phase HOF (HOF_{Solid}) because it is related directly with the detonation characteristics. According to Hess' law, solid phase HOF can be obtained by,

$$HOF_{Solid} = HOF_{Gas} - HOF_{Sub} \quad (1)$$

where HOF_{Sub} is the heat of sublimation and can be evaluated by the Byrd and Rice method[2] in the framework of the Politzer approach,[3] using the following empirical relation,

$$HOF_{Sub} = \beta_1 A^2 + \beta_2(v\sigma^2_{tot}) + \beta_3 \quad (2)$$

where A is the area of the isosurface of 0.001 electrons/bohr^3 electronic density, v indicates the degree of balance between the positive and negative surface potentials, σ^2_{tot} is a measure of variability of the electrostatic potential, and β_1, β_2, and β_3 are determined through a least-squares with the experimental HOF_{Solid} of a selected set of known materials.[2] Surface area, degree of balance between the positive and negative surface potentials and variability of the electrostatic potential are calculated using WFA program.[4]

The lattice potential energies and lattice energies were predicted using Jenkins approach.[5] In the Jenkins equation[5d] for the 1:3 salts the *generalised* parameters α and β were utilized with appropriate ionic strength values, I = 6. Based on a Born-Haber cycle (Fig. 1), the heat of formation of a salt can be simplified by the formula,

$$HOF\ (salt, 298\ K) = HOF\ (cation, 298\ K) + HOF\ (anion, 298\ K) - H_L \qquad (3)$$

where H_L is the lattice enthalpy of the ionic salts. HOF of an ionic compound can be simplified by subtracting the lattice energy of the salt (H_L) from the sum of the HOFs of the cation and anion according to Equation (3). The HOF of the cations and anions were computed by using the method of isodesmic reactions. The lattice enthalpy (H_L) could be predicted by the formula suggested by Jenkins et al.[5a] using its lattice potential energy (U_{POT}, kJ/mol) as,

$$H_L = U_{POT} + 2RT \text{ for 1:1 salt} \qquad (4)$$

$$H_L = U_{POT} + 3RT \text{ for 2:1 salt} \qquad (5)$$

$$H_L = U_{POT} + 4RT \text{ for 3:1 salt} \qquad (6)$$

The lattice potential energy U_{POT} (kJ/mol) can be predicted from four different approaches as suggested by Jenkins et al.[5b,c] using following equations,

$$U_{POT} = AI(2I/V)^{1/3} \qquad (7)$$

$$U_{POT} = B(I^4\rho/M)^{1/3} \qquad (8)$$

$$U_{POT} = \gamma(\rho/M)^{1/3} + \delta \qquad (9)$$

$$U_{POT} = 2I[\alpha(V)^{-1/3} + \beta] \qquad (10)$$

In above equations (7-10), I is the ionic strength, ρ is the density (g/cm^3), V is the estimated volume of ionic material (nm^3), M is the chemical formula mass of the ionic material (g/mol), and the coefficients A, B, γ (kJ/mol.cm), δ (kJ/mol), α, and β are taken from the literature.[5] Equations (9) and (10) are used to calculate the lattice potential energy for salts with 1:1 and 2:1 charge ratio. Equation (7) is normally employed for salts likely to have lattice energy greater than 5000 kJ/mol but it seems to work quite well in this case and for these materials.

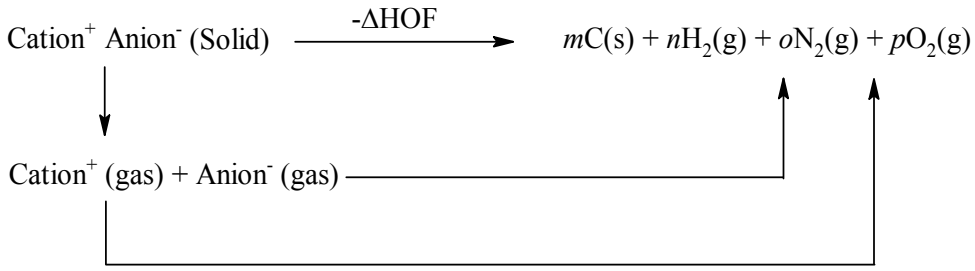

Figure 1. Born-Haber cycle for the formation of energetic salts.

The empirical Kamlet-Jacobs[6] equations were employed to estimate the values of *D* and *P* for the high energy materials containing C, H, O and N as following equations:

$$D = 1.01(NM^{0.5}Q^{0.5})^{0.5}(1 + 1.30\rho_o) \quad (11)$$

$$P = 1.55\rho_o{}^2 NM^{0.5}Q^{0.5} \quad (12)$$

where in above equations *D* is detonation velocity (km/s), *P* is detonation pressure (GPa), N is moles of gaseous detonation products per gram of explosives, M is average molecular weights of gaseous products, *Q* is chemical energy of detonation (cal/g) defined as the difference of the HOFs between products and reactants, and ρ_o is the density of explosive (g/cm^3).

References

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(5) (a) Jenkins, H. D. B. *J. Chem. Educ.* **2005**, *82*, 950. (b) Jenkins, H. D. B.; Tudela, D.; Glasser, L. *Inorg. Chem.* **2002**, *41*, 2364. (c) Glasser, L.; Jenkins, H. D. B. *J. Am. Chem. Soc.*

2000, *122*, 632. (d) Jenkins, H. D. B.; Roobottom, H. K.; Passmore, J.; Glasser, L. *Inorg. Chem.* **1999**, *38*, 3609.

(6) (a) Kamlet, M. J.; Jacobs, S. J. *J. Chem. Phys.* **1968**, *48*, 23. (b) Kamlet, M. J.; Ablard, J. E. *J. Chem. Phys.* **1968**, *48*, 36.

Experimental data

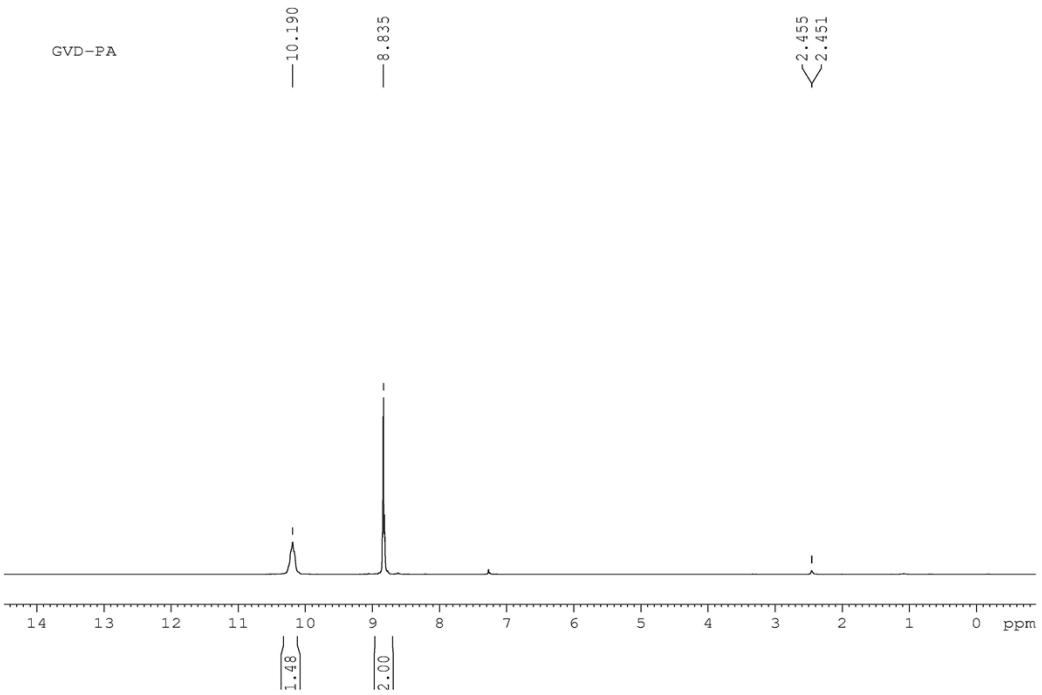
1	Picric acid a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
2	4*H*-1,2,4-Triazol-4-aminium 2,4,6-trinitrophenolate (1a) a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
3	3-Amino-1*H*-1,2,4-triazol-4-ium-2,4,6-trinitrophenolate (1b) a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
4	3,5-Diamino-1*H*-1,2,4-triazol-4-ium-2,4,6-trinitrophenolate (1c) a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
5	3,4-Diamino-1,2,5-oxadiazol-2-ium 2,4,6-trinitrophenolate (1d) a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA
6	Diaminomethaniminium-2,4,6-trinitrophenolate (1e) a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
7	2,4,6-Trinitro-m-cresol a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA
8	4*H*-1,2,4-Triazol-4-aminium 3-methyl-2,4,6-trinitrophenolate (2a) a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA
9	3-Amino-1*H*-1,2,4-triazol-4-ium 3-methyl-2,4,6-trinitrophenolate (2b) a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
10	3,5-Diamino-1*H*-1,2,4-triazol-4-ium 3-methyl-2,4,6-trinitrophenolate (2c) a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA

11	3,4-Diamino-1,2,5-oxadiazol-2-ium 3-methyl-2,4,6-trinitrophenolate (2d) a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA
12	Diaminomethaniminium 3-methyl-2,4,6-trinitrophenolate (2e) a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
13	3-Azido-2,4,6-trinitrophenol a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA
14	3-Amino-1H-1,2,4-triazol-4-ium 3-azido-2,4,6-trinitrophenolate (3b) a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
15	3,5-Diamino-1H-1,2,4-triazol-4-ium 3-azido-2,4,6-trinitrophenolate (3c) a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
16	3,4-Diamino-1,2,5-oxadiazol-2-ium 3-azido-2,4,6-trinitrophenolate (3d) a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
17	Diaminomethaniminium 3-azido-2,4,6-trinitrophenolate (3e) a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
18	Styphnic acid a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
19	Bis(3-amino-1H-1,2,4-triazol-4-ium) 2,4,6-trinitrobenzene-1,3-diolate (4b) a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA
20	Bis(3,5-diamino-1H-1,2,4-triazol-4-ium) 2,4,6-trinitrobenzene-1,3-diolate (4c) a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA
21	Bis(3,4-diamino-1,2,5-oxadiazol-2-ium) 2,4,6-trinitrobenzene-1,3-diolate (4d) a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA

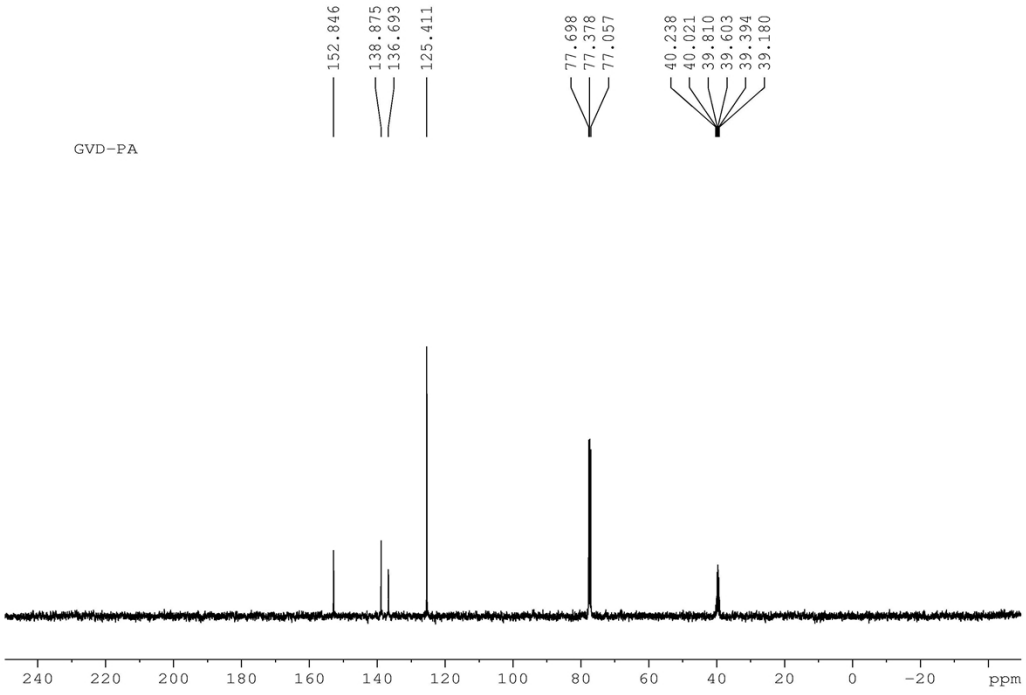
22	Bis(diaminomethaniminium) 2,4,6-trinitrobenzene-1,3-diolate (4e) a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA
23	2,4,6-Trinitro-1,3,5-benzenetriol a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
24	Tris(4H-1,2,4-triazol-4-aminium) 2,4,6-trinitrobenzene-1,3,5-triolate (5a) a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA
25	Tris(3-amino-1H-1,2,4-triazol-4-ium) 2,4,6-trinitrobenzene-1,3,5-triolate (5b) a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA
26	Tris(3,5-diamino-1H-1,2,4-triazol-4-ium) 2,4,6-trinitrobenzene-1,3,5-triolate (5c) a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
27	Tris(3,4-diamino-1,2,5-oxadiazol-2-ium) 2,4,6-trinitrobenzene-1,3,5-triolate (5d) a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA
28	Tris(diaminomethaniminium) 2,4,6-trinitrobenzene-1,3,5-triolate (5e) a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA

1. **Picric acid**

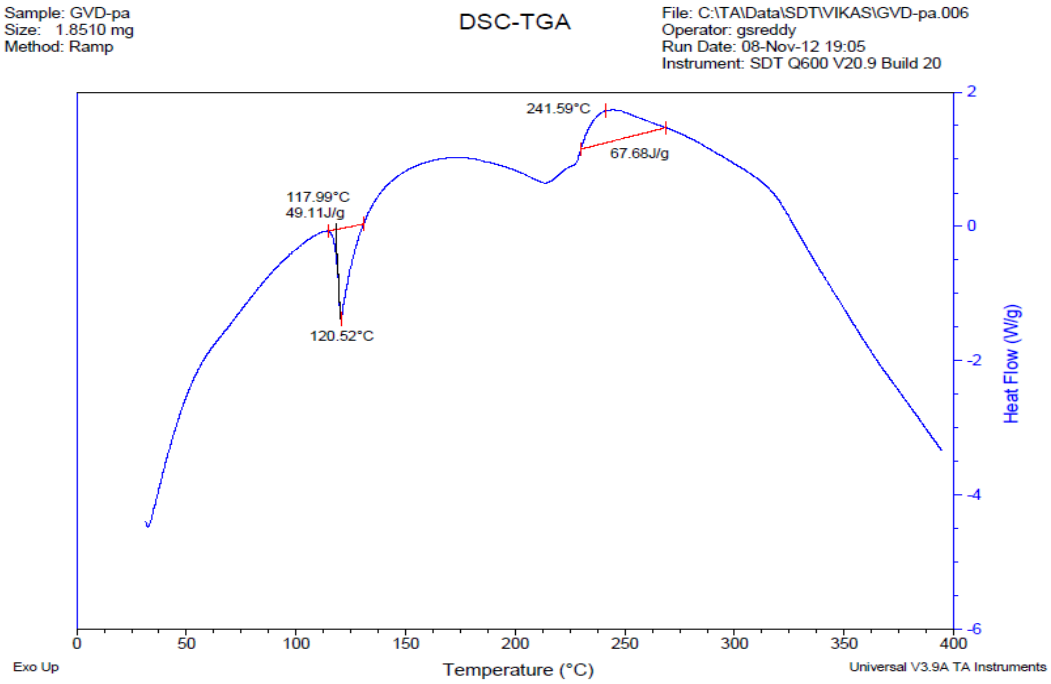
1a. ^{1}H NMR



1b. ^{13}C NMR

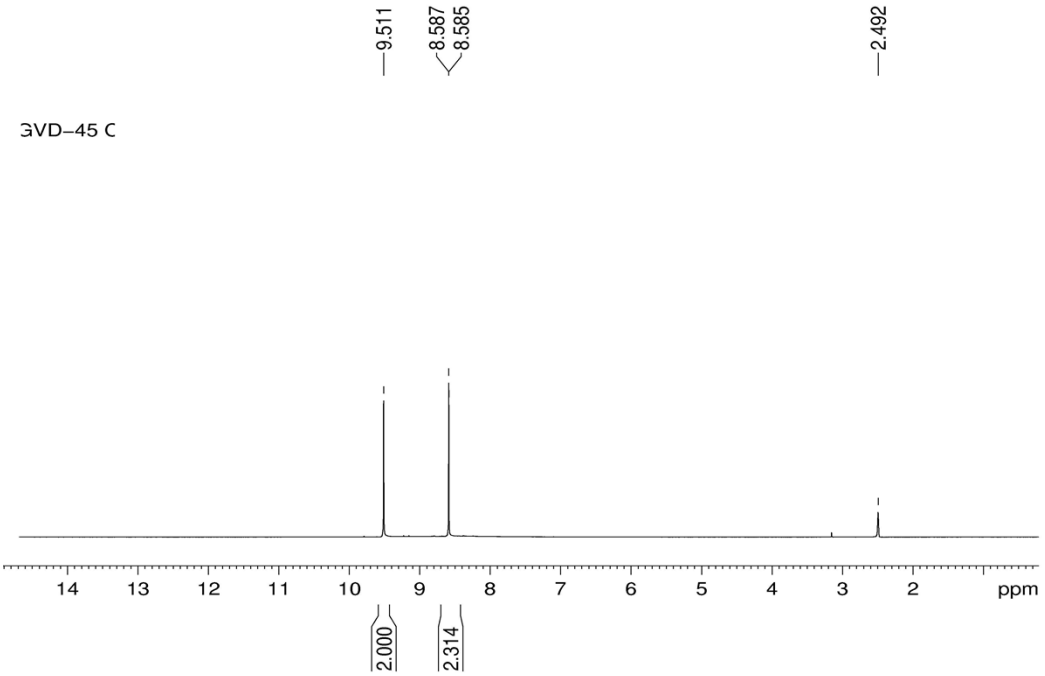


1c. TG-DTA

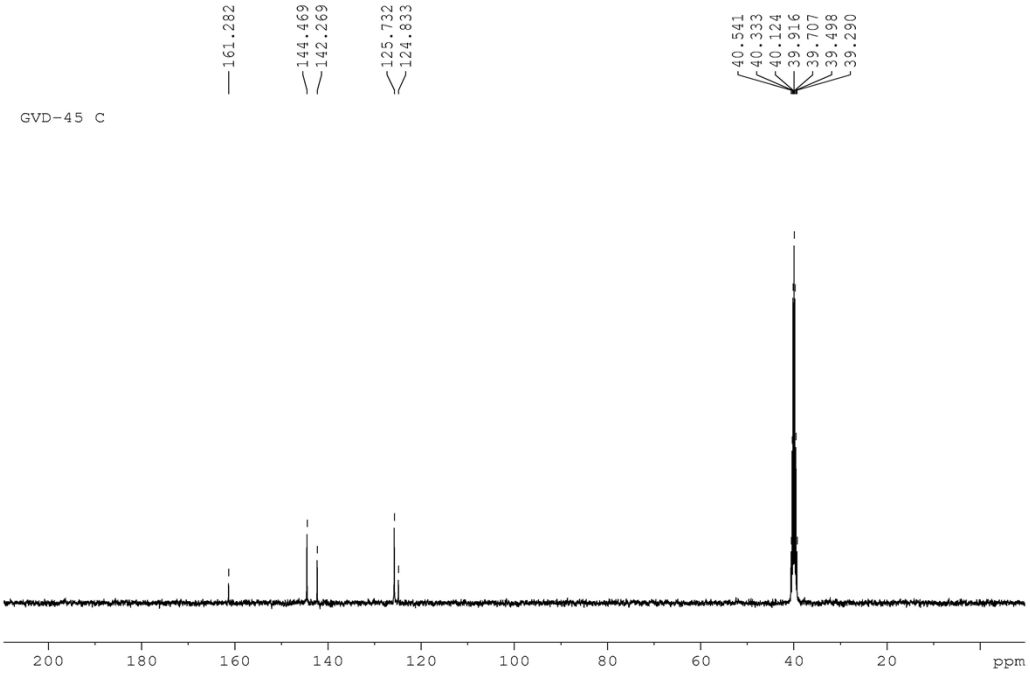


2. 4*H*-1,2,4-Triazol-4-aminium 2,4,6-trinitrophenolate (1a)

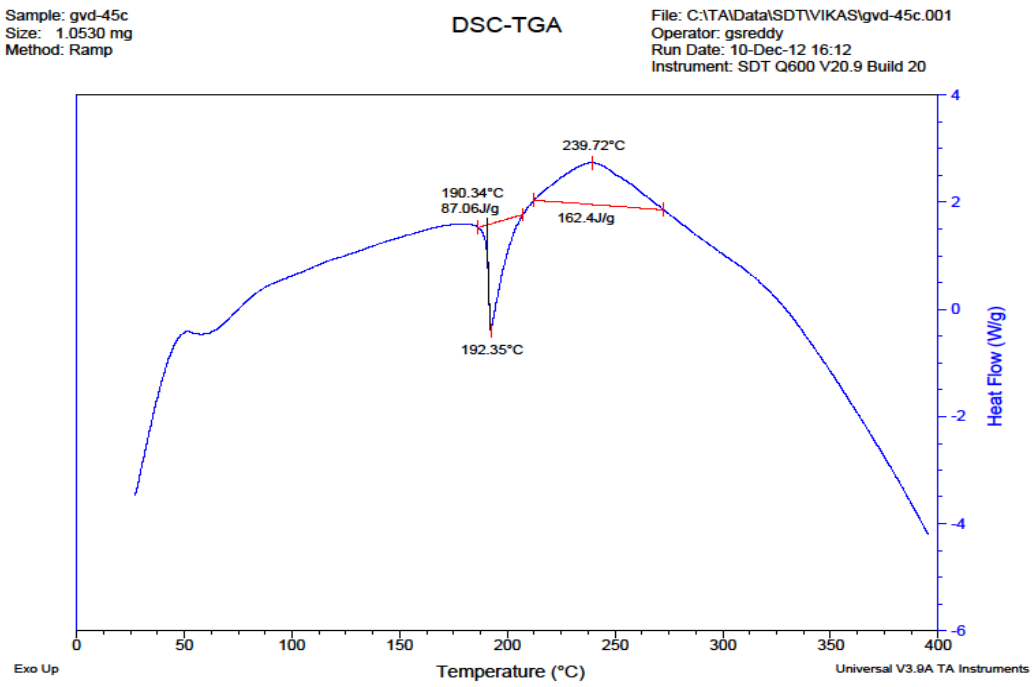
2a. ^{1}H NMR



2b. ^{13}C NMR

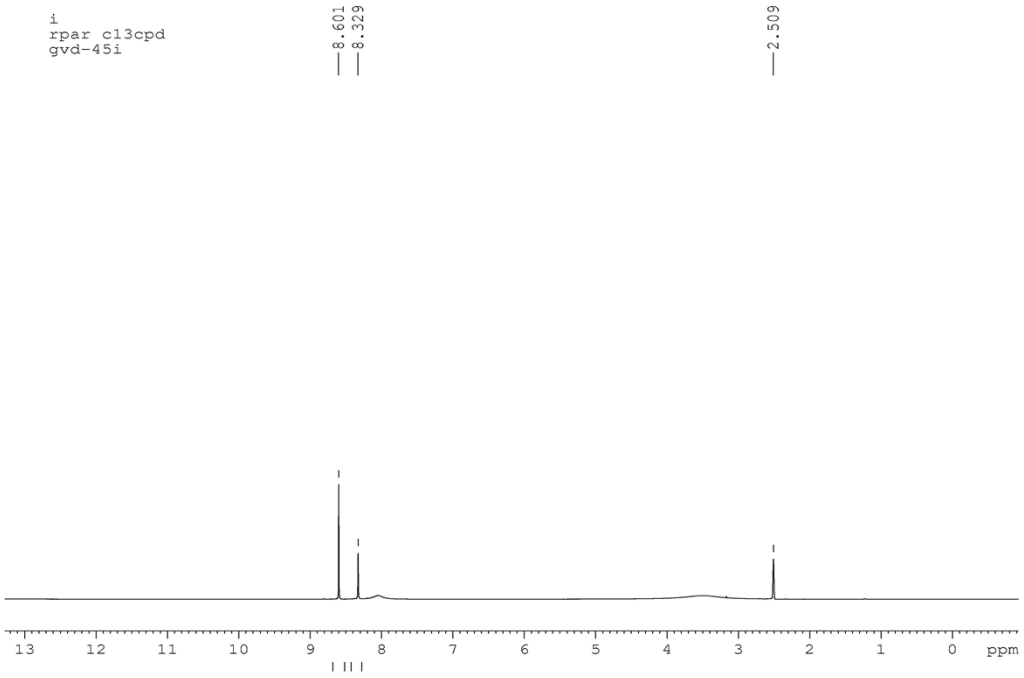


2c. TG-DTA

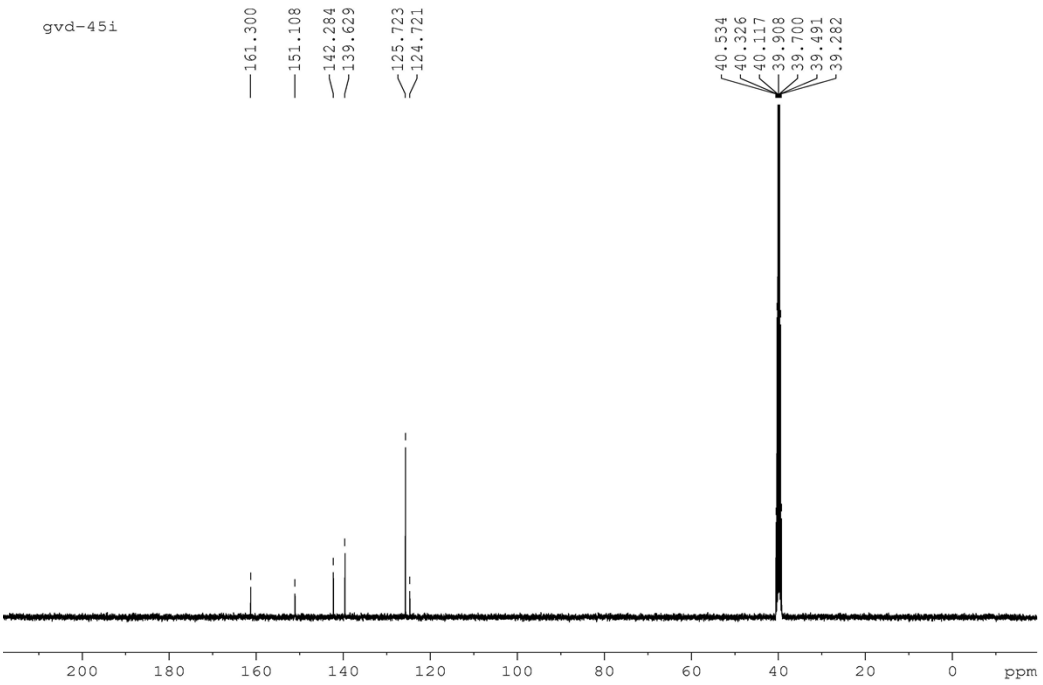


3. **3-Amino-1*H*-1,2,4-triazol-4-ium-2,4,6-trinitrophenolate (1b)**

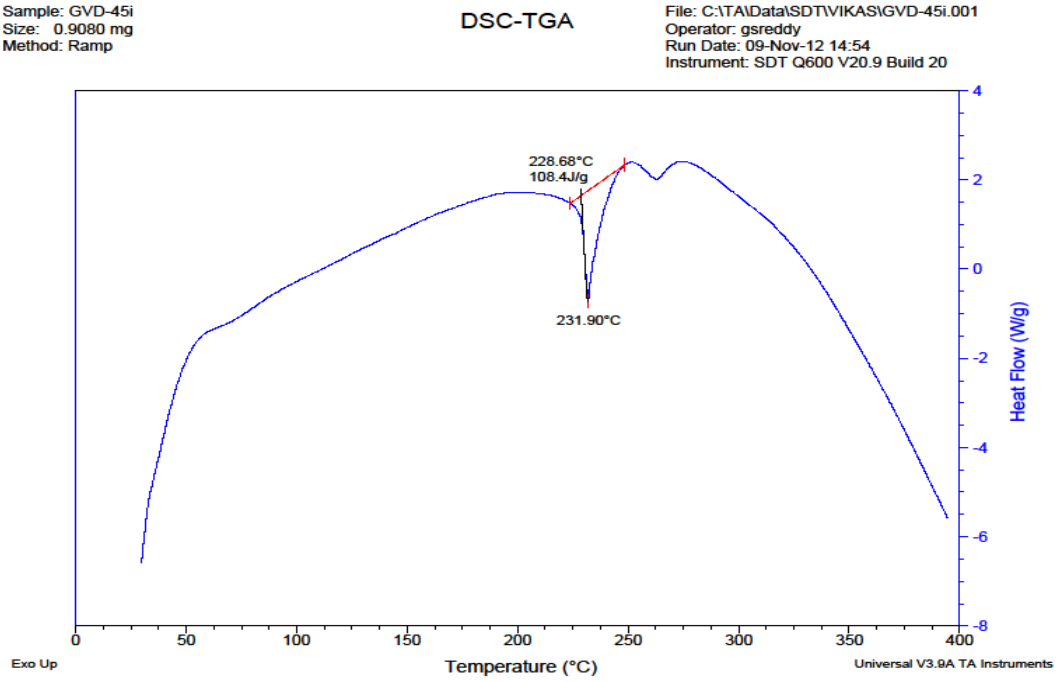
3a. ^{1}H NMR



3b. ^{13}C NMR

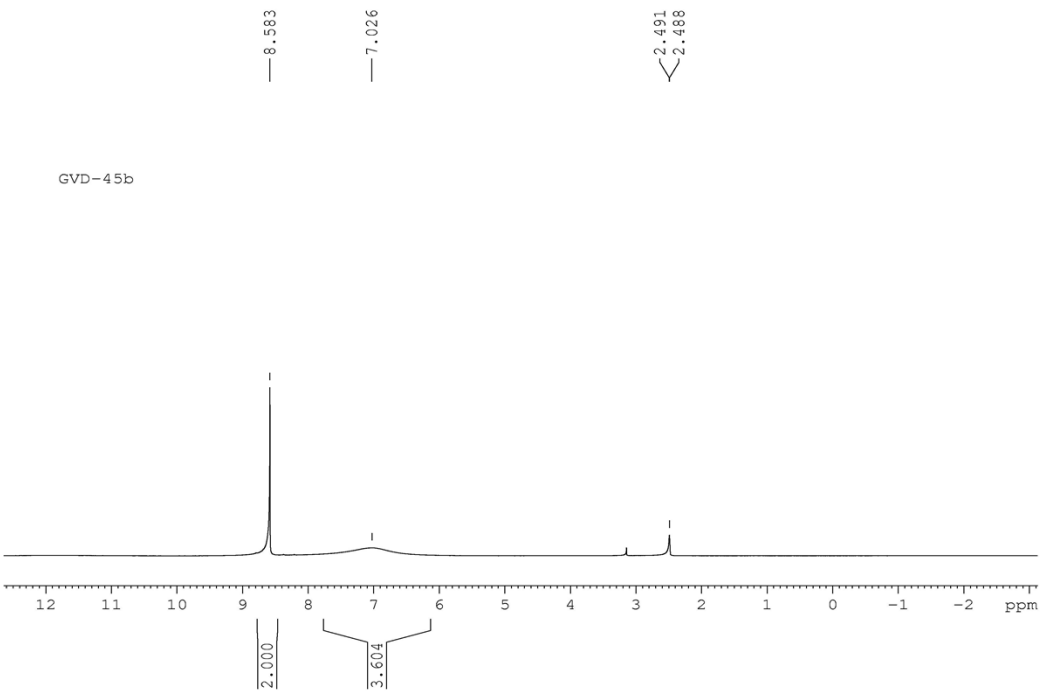


3c. TG-DTA

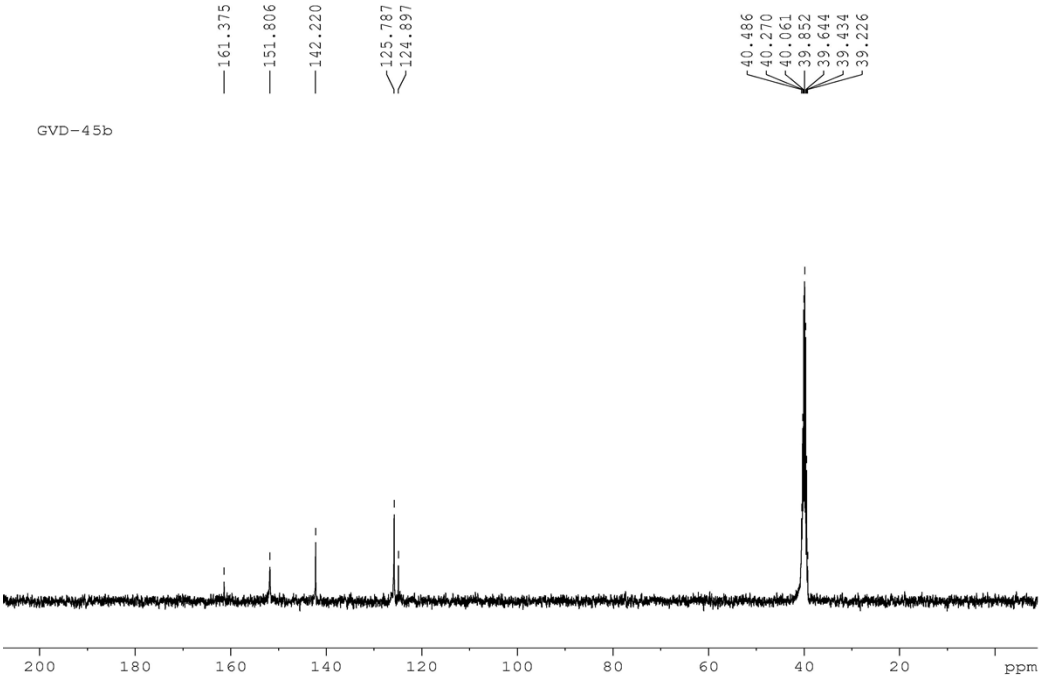


4. **3,5-Diamino-1*H*-1,2,4-triazol-4-ium-2,4,6-trinitrophenolate (1c)**

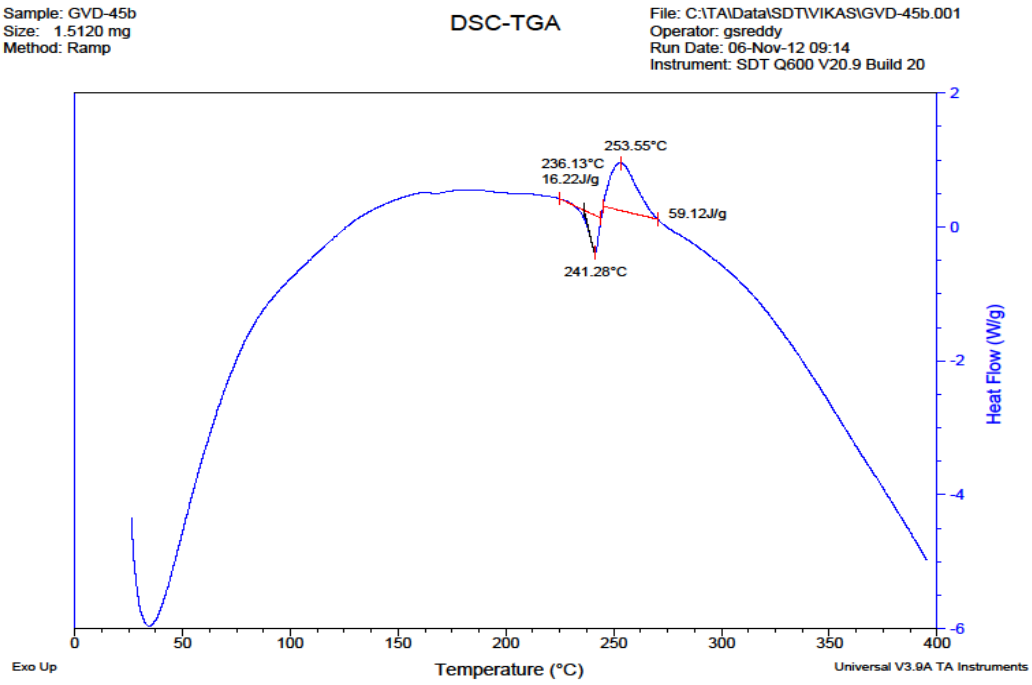
4a. ^{1}H NMR



4b. ^{13}C NMR

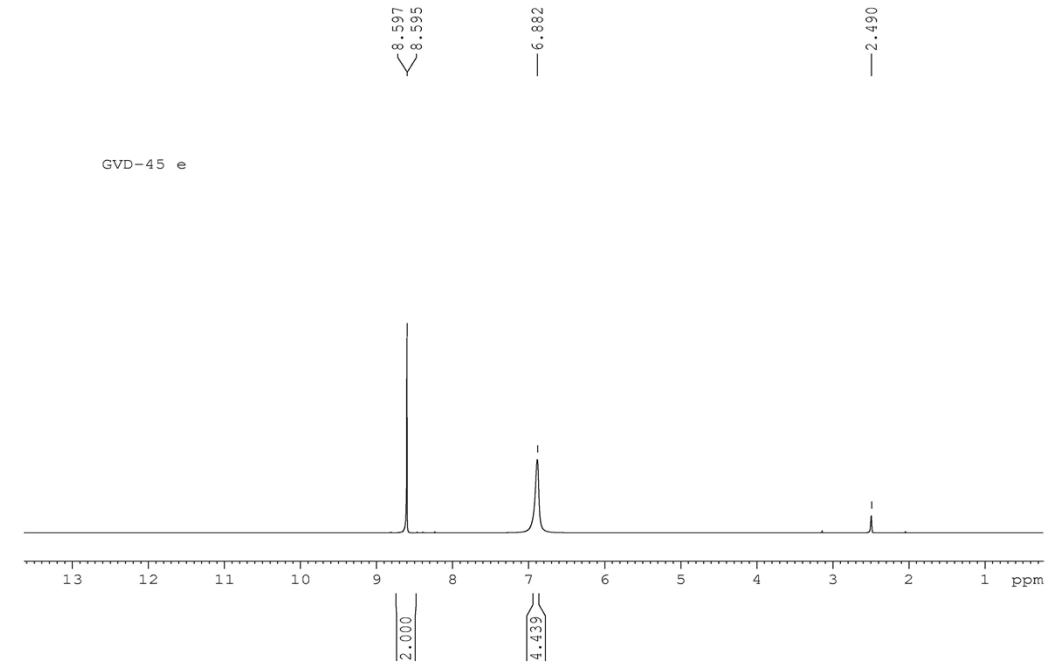


4d. TG-DTA

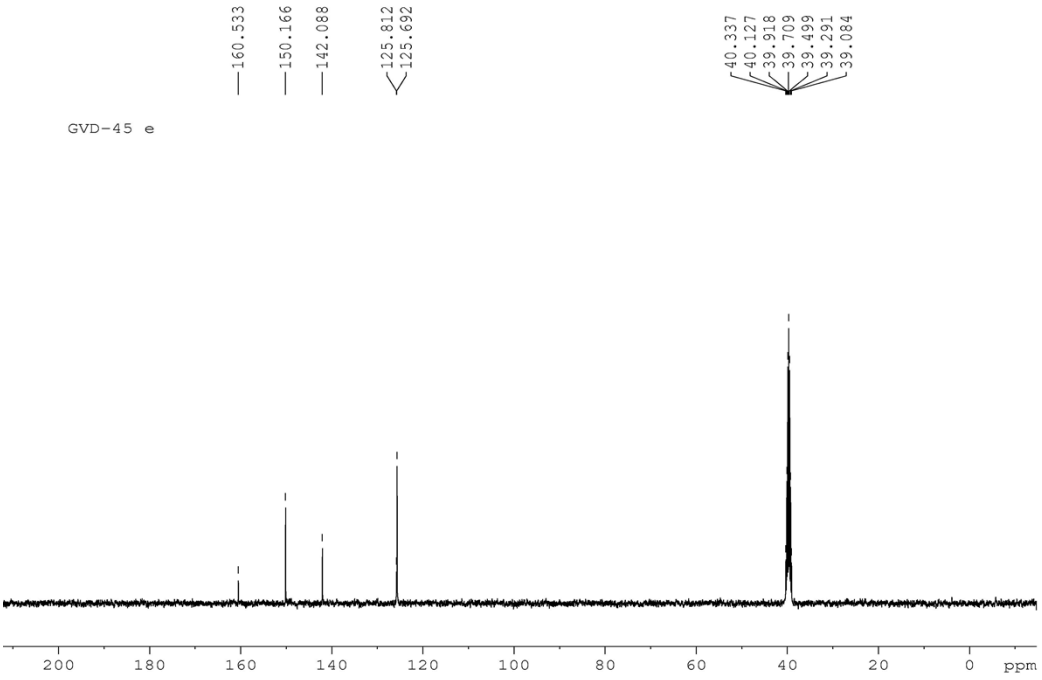


5. **3,4-Diamino-1,2,5-oxadiazol-2-ium 2,4,6-trinitrophenolate (1d)**

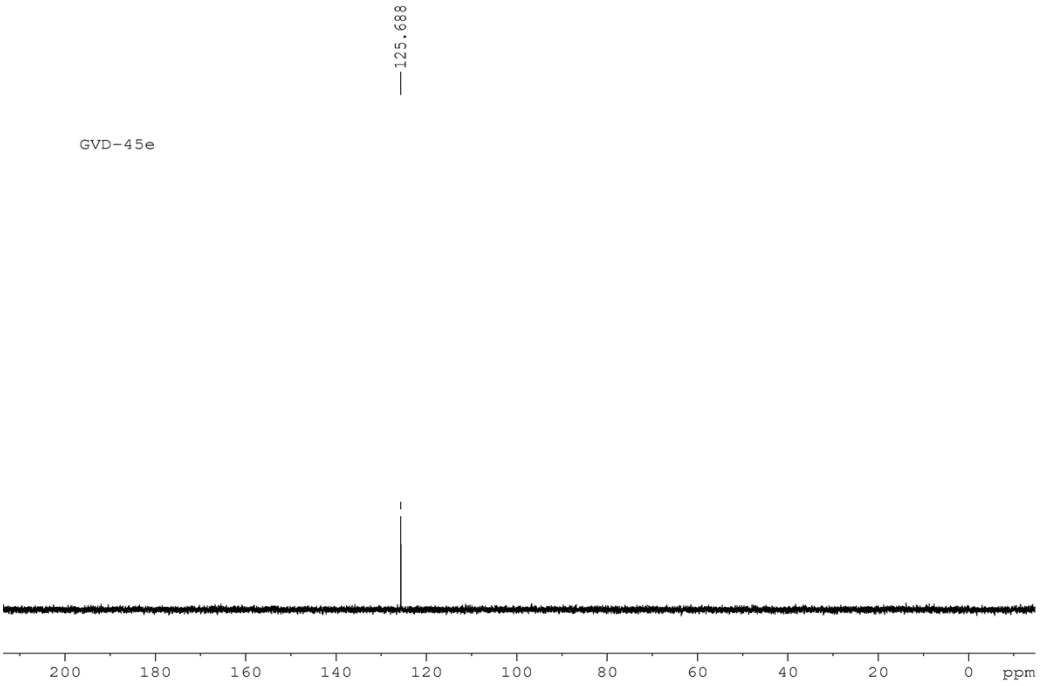
5a. ^{1}H NMR



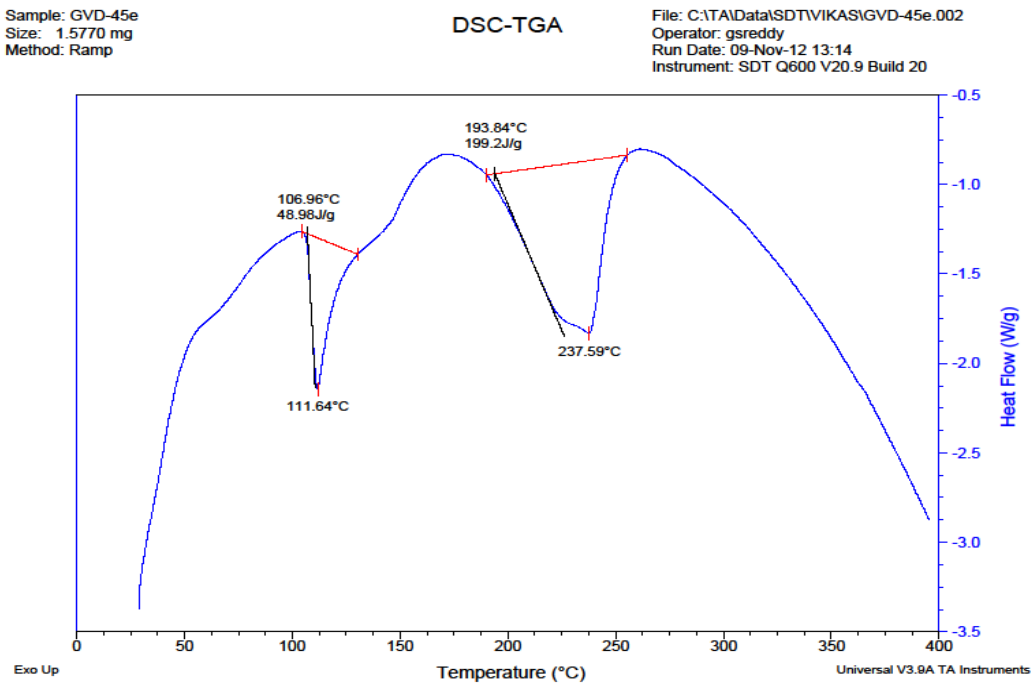
5b. ^{13}C NMR



5c. DEPT

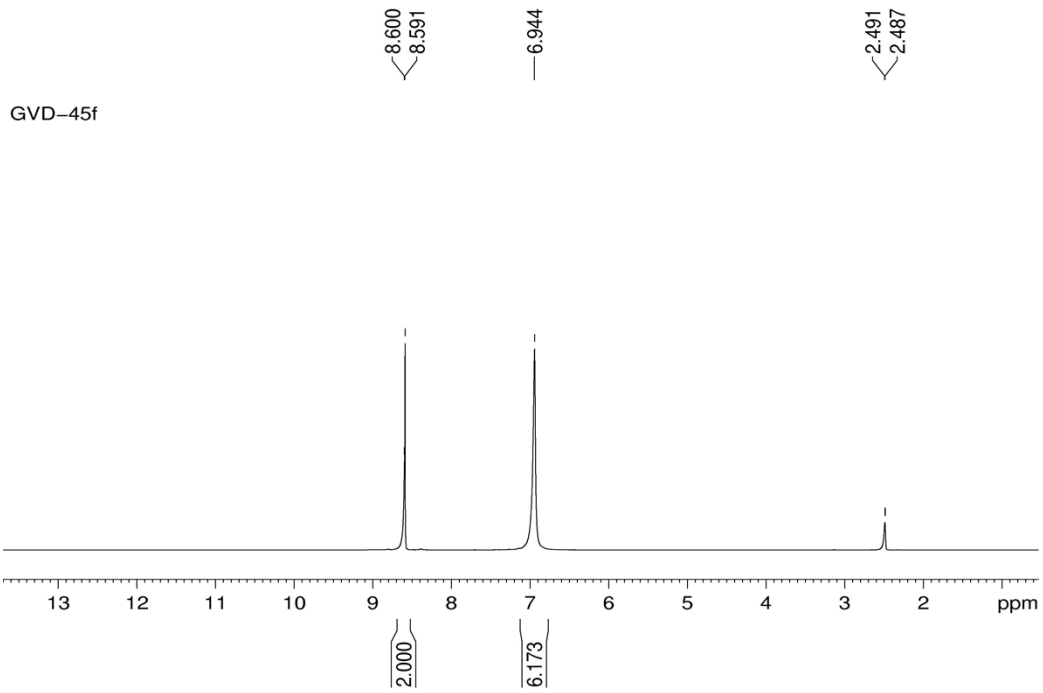


5d. TG-DTA

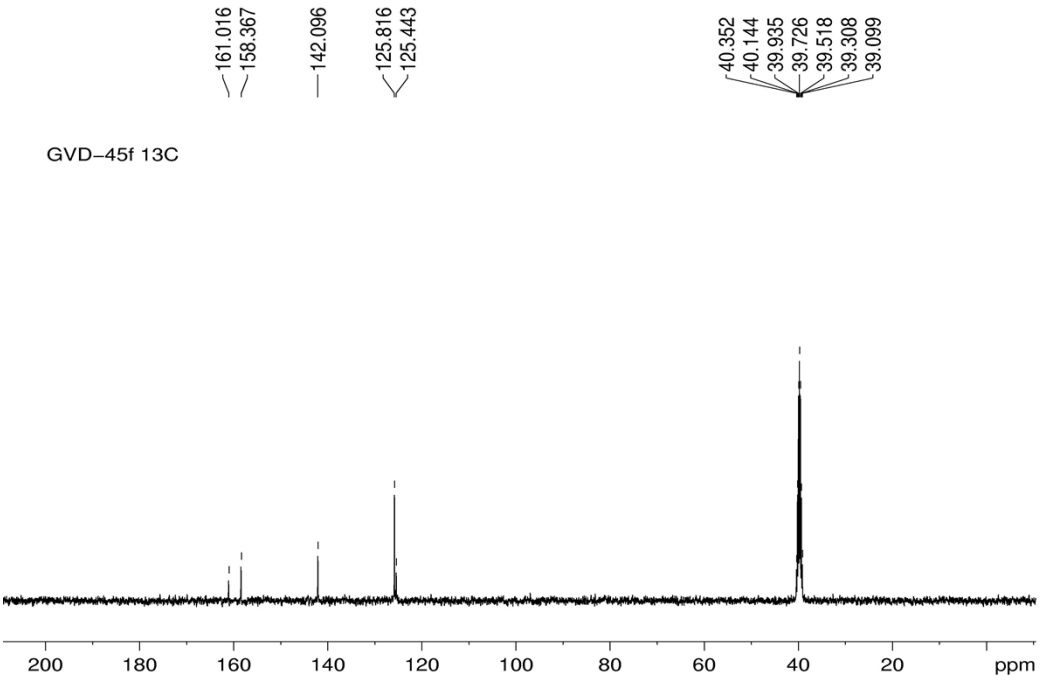


6. **Diaminomethaniminium-2,4,6-trinitrophenolate (1e)**

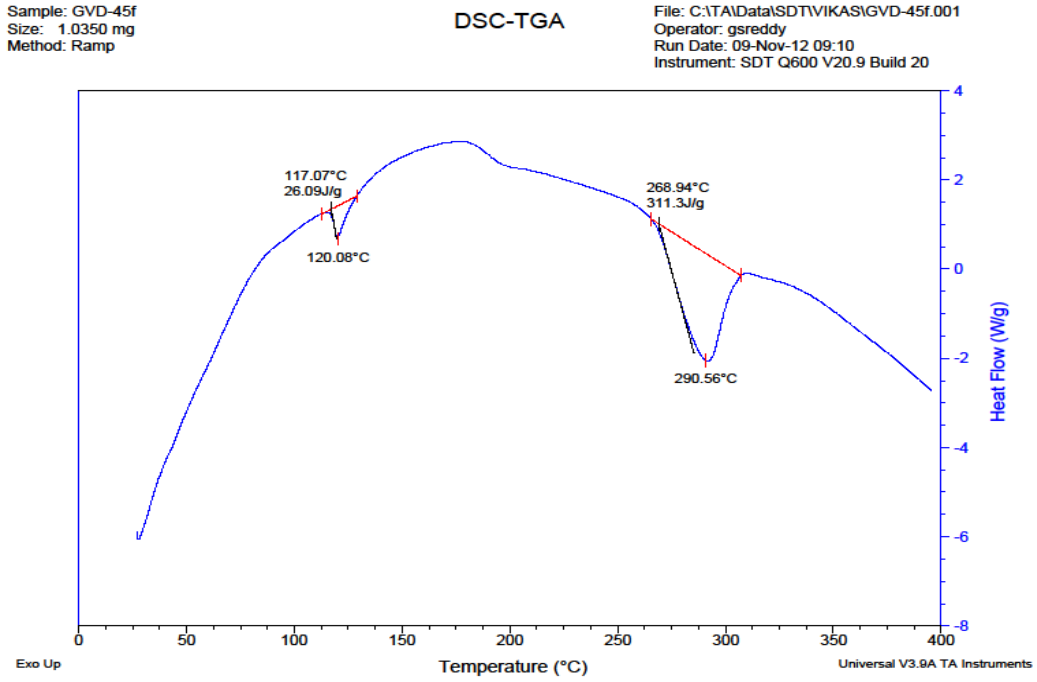
6a. ^{1}H NMR



6b. ^{13}C NMR

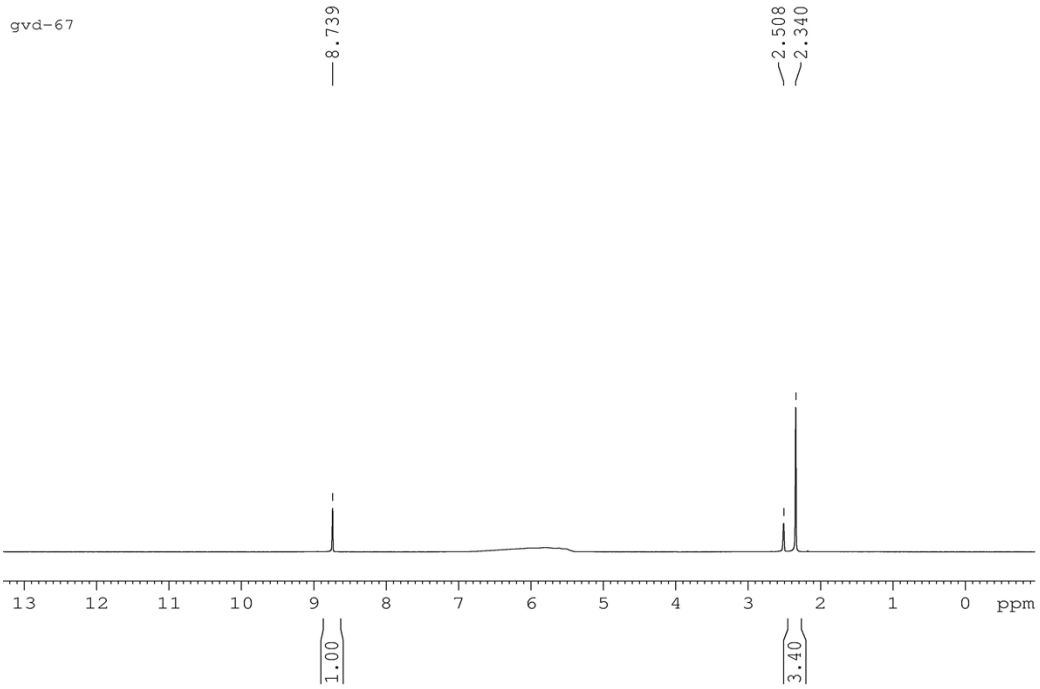


6c. TG-DTA

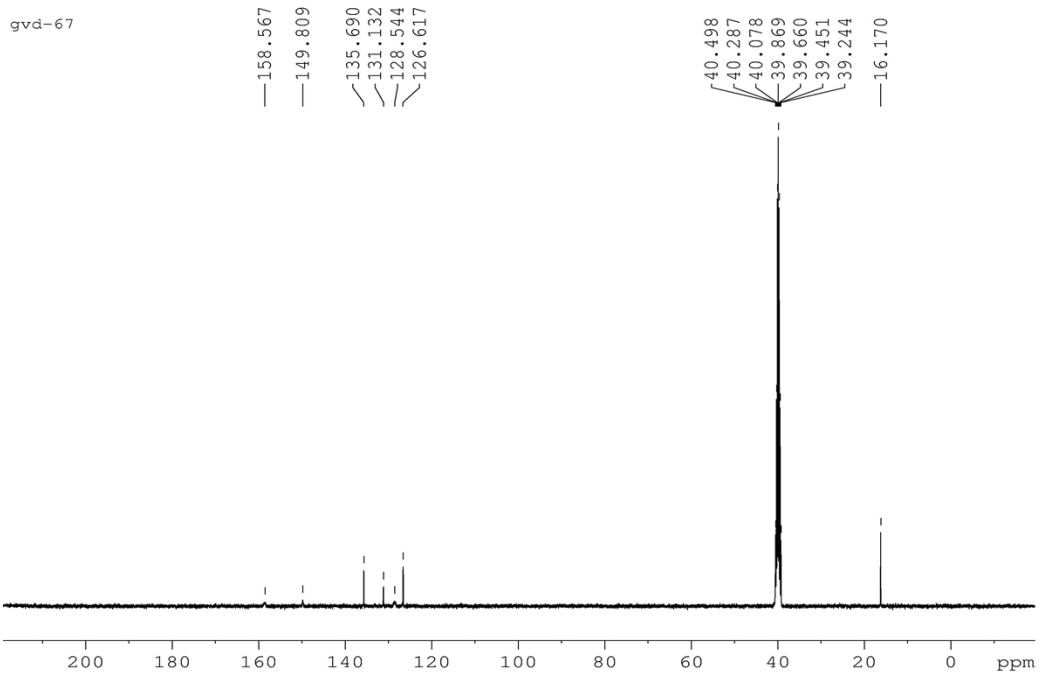


7. **2,4,6-Trinitro-m-cresol**

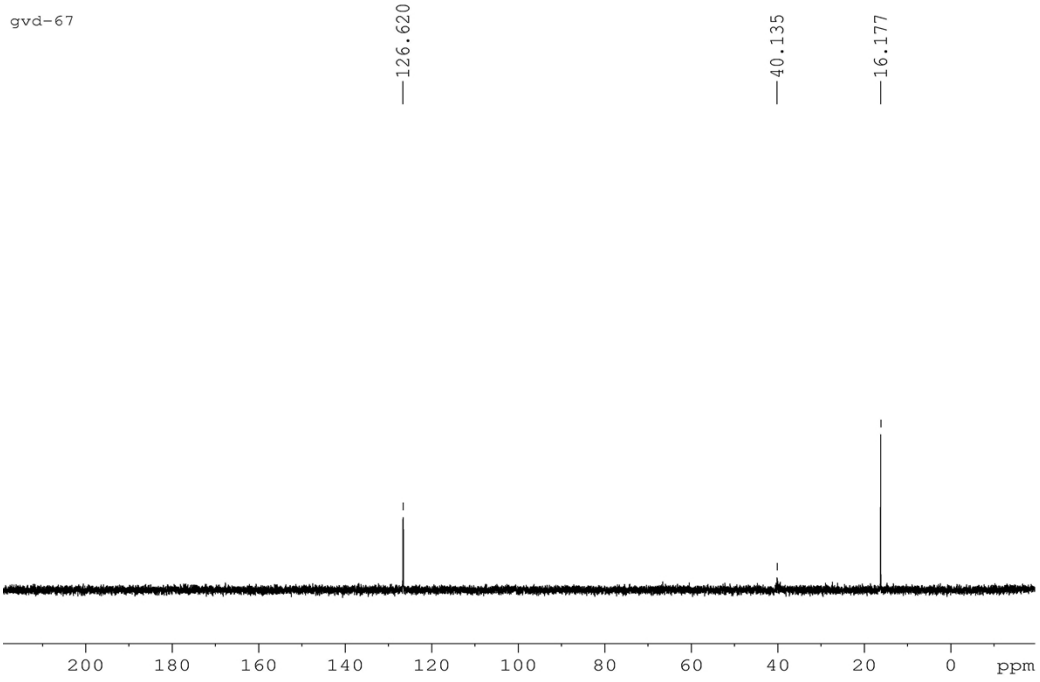
7a. ^{1}H NMR



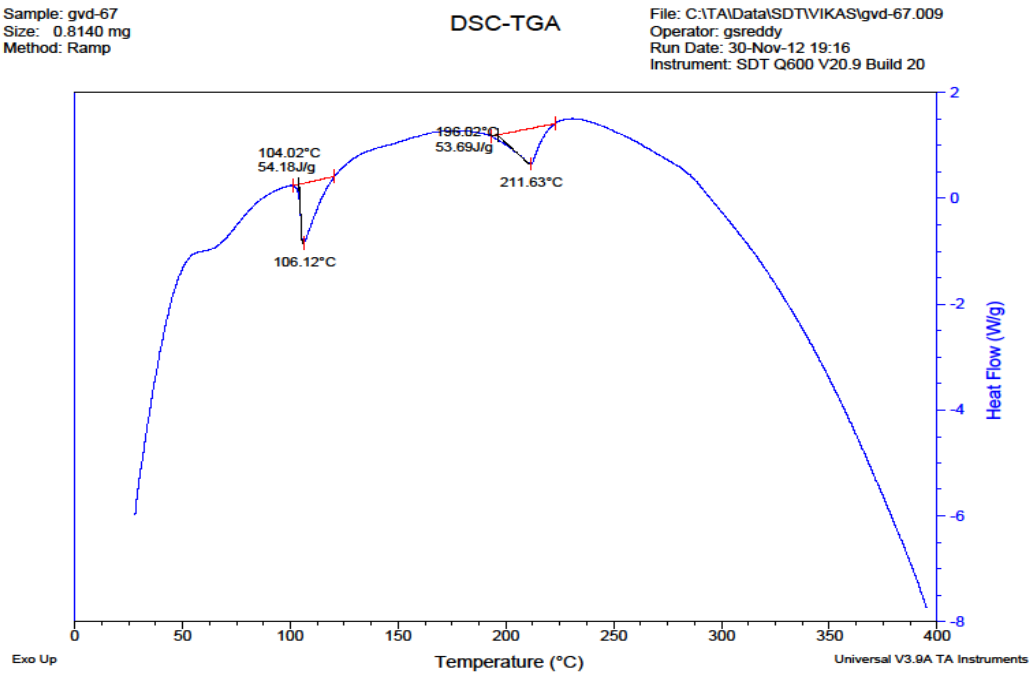
7b. ^{13}C NMR



7c. DEPT

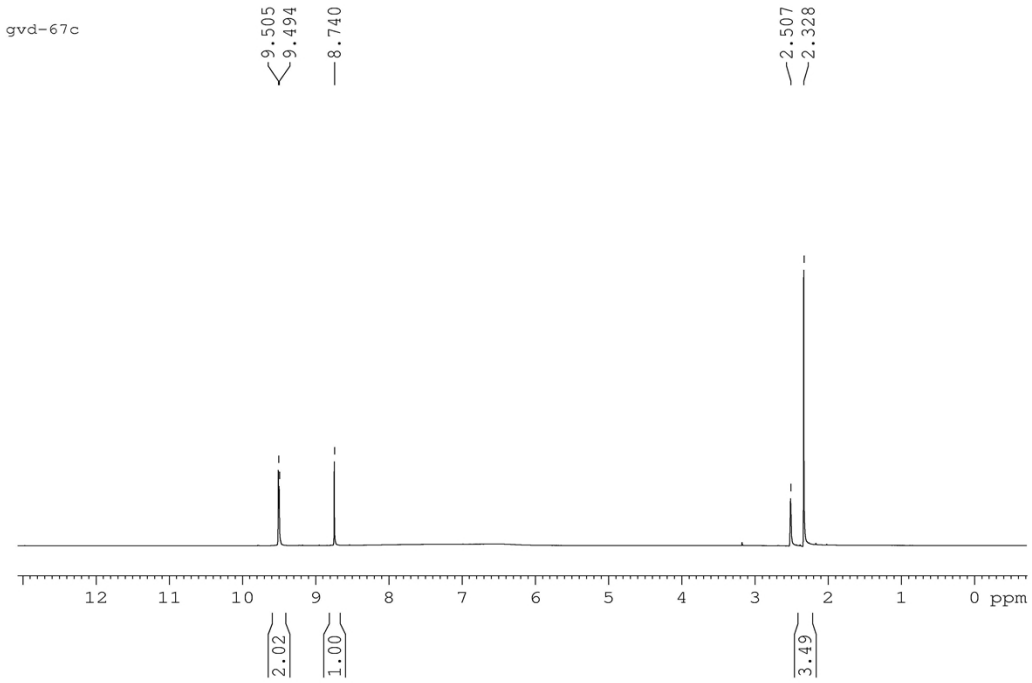


7d. TG-DTA

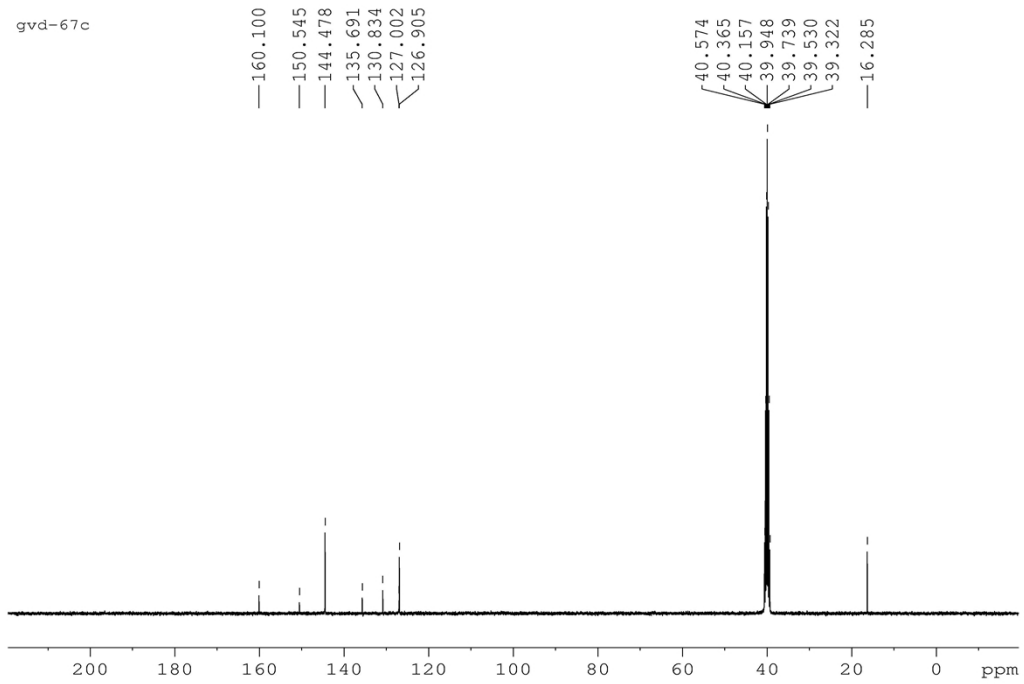


8. **4*H*-1,2,4-Triazol-4-aminium 3-methyl-2,4,6-trinitrophenolate (2a)**

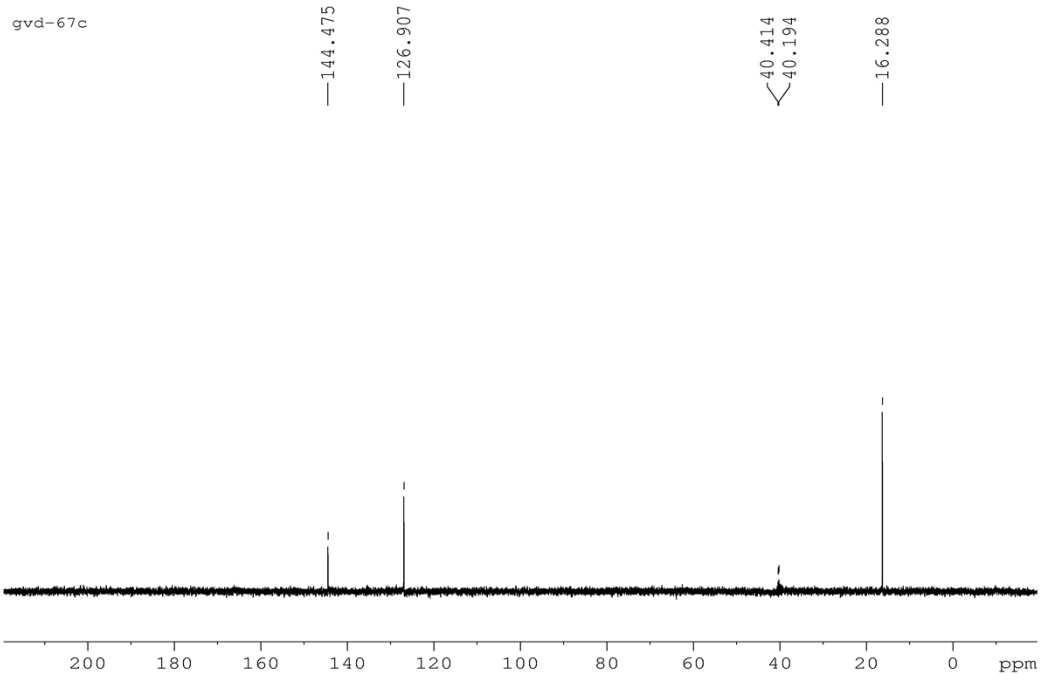
8a. ^{1}H NMR



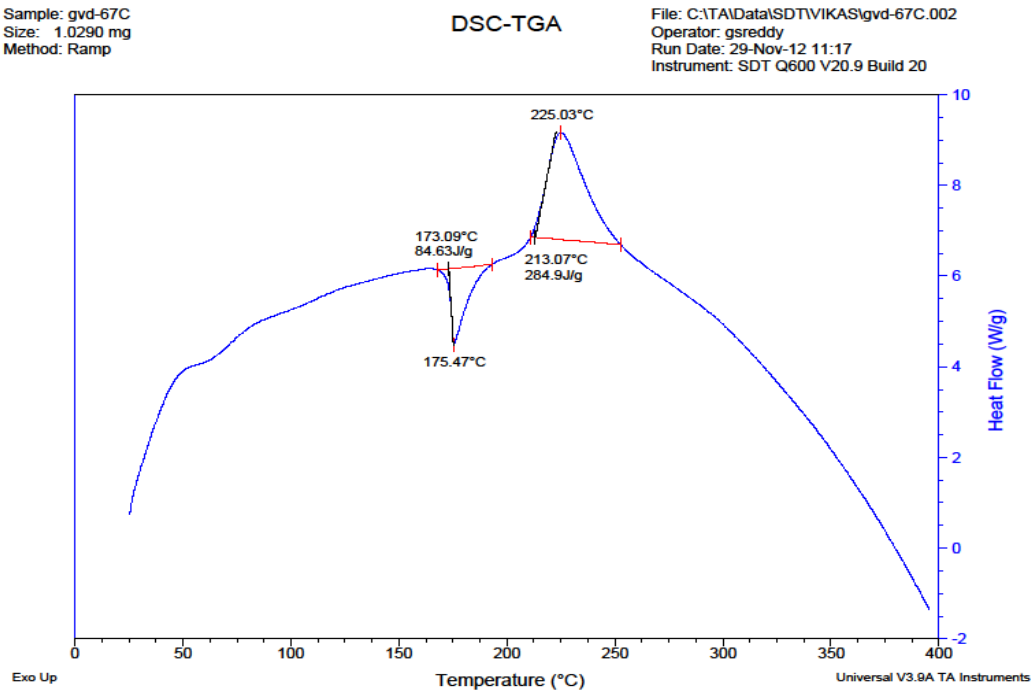
8b. ^{13}C NMR



8c. DEPT

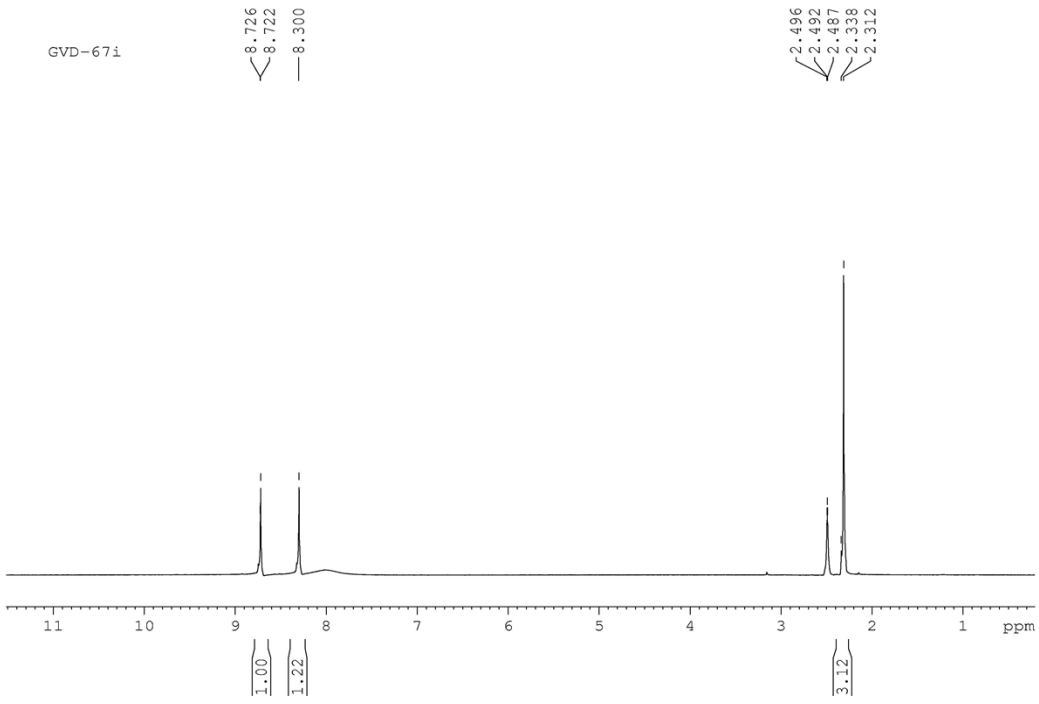


8d. TG-DTA

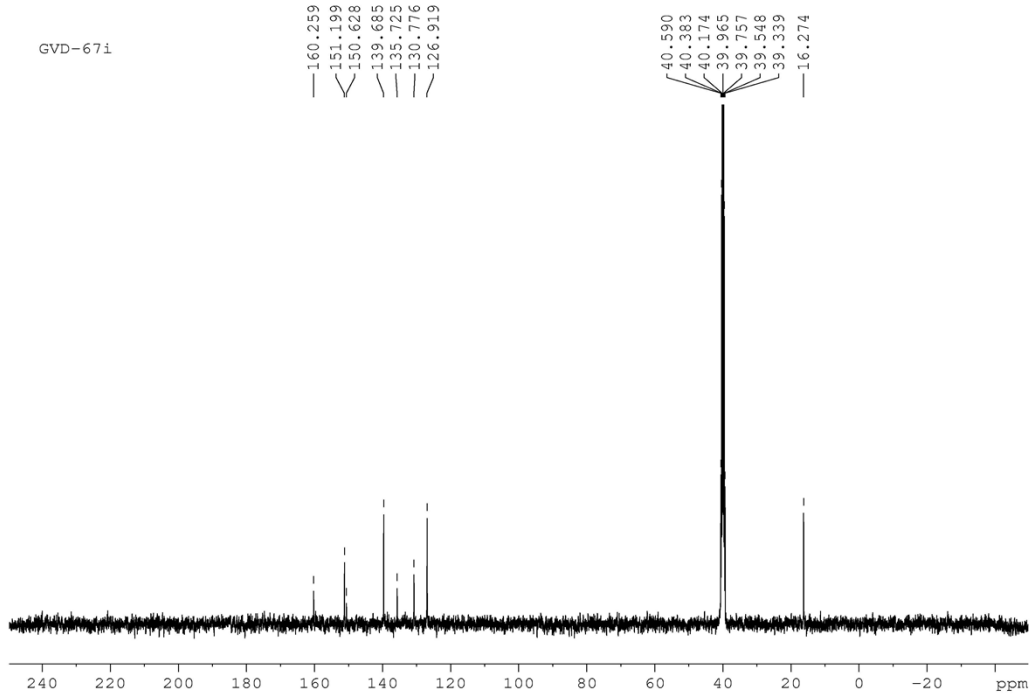


9. **3-Amino-1*H*-1,2,4-triazol-4-ium 3-methyl-2,4,6-trinitrophenolate (2b)**

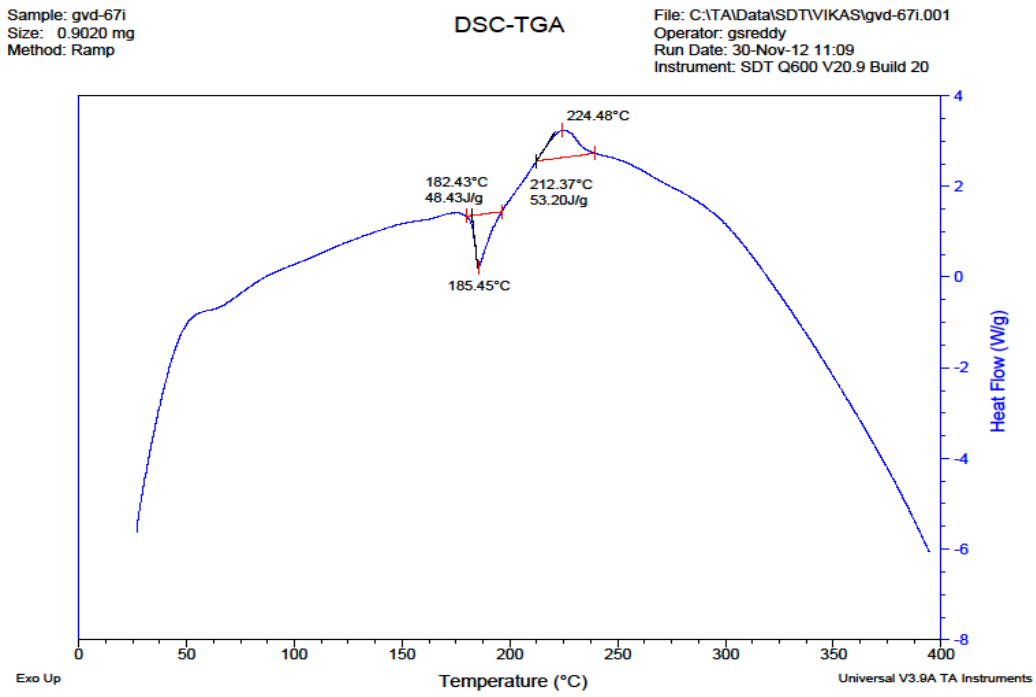
9a. ^{1}H NMR



9b. ^{13}C NMR

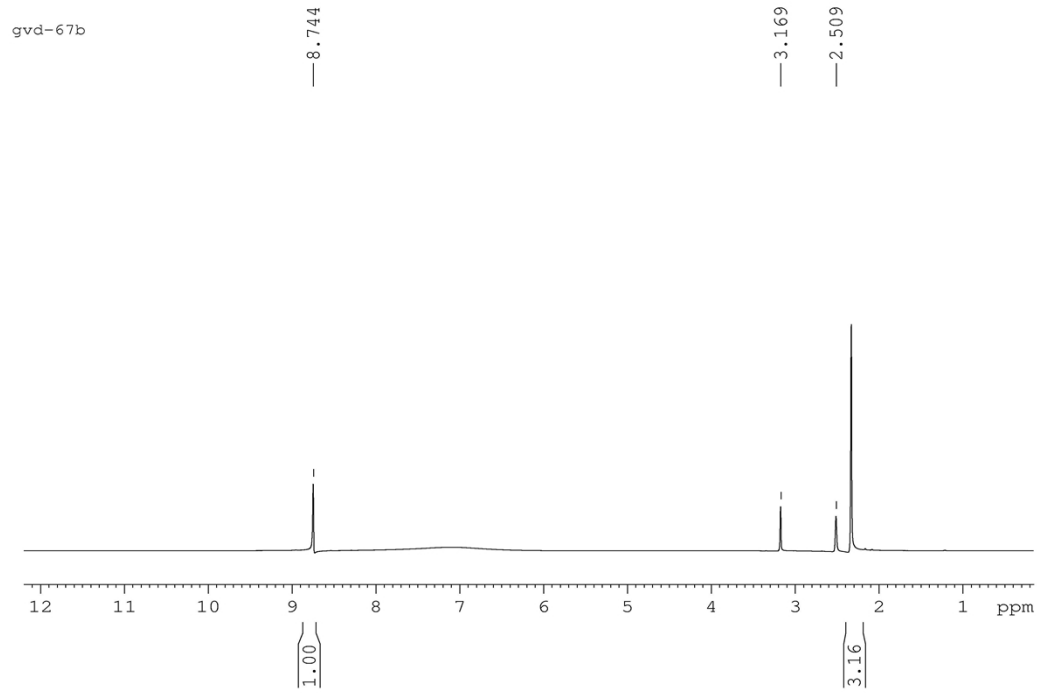


9c. TG-DTA

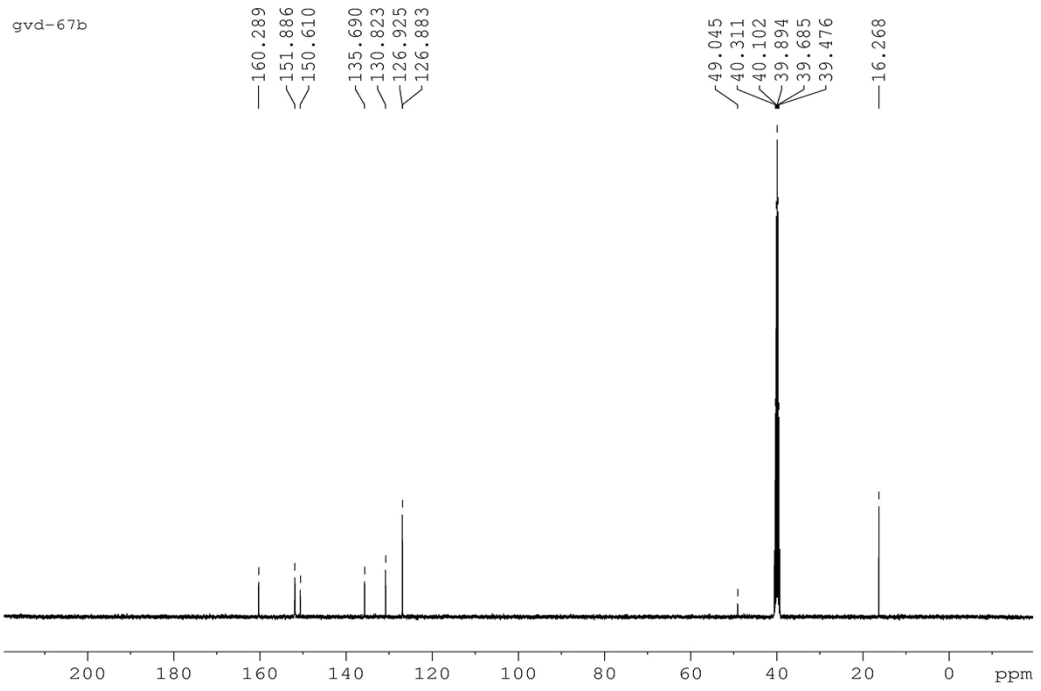


10. **3,5-Diamino-1*H*-1,2,4-triazol-4-ium 3-methyl-2,4,6-trinitrophenolate (2c)**

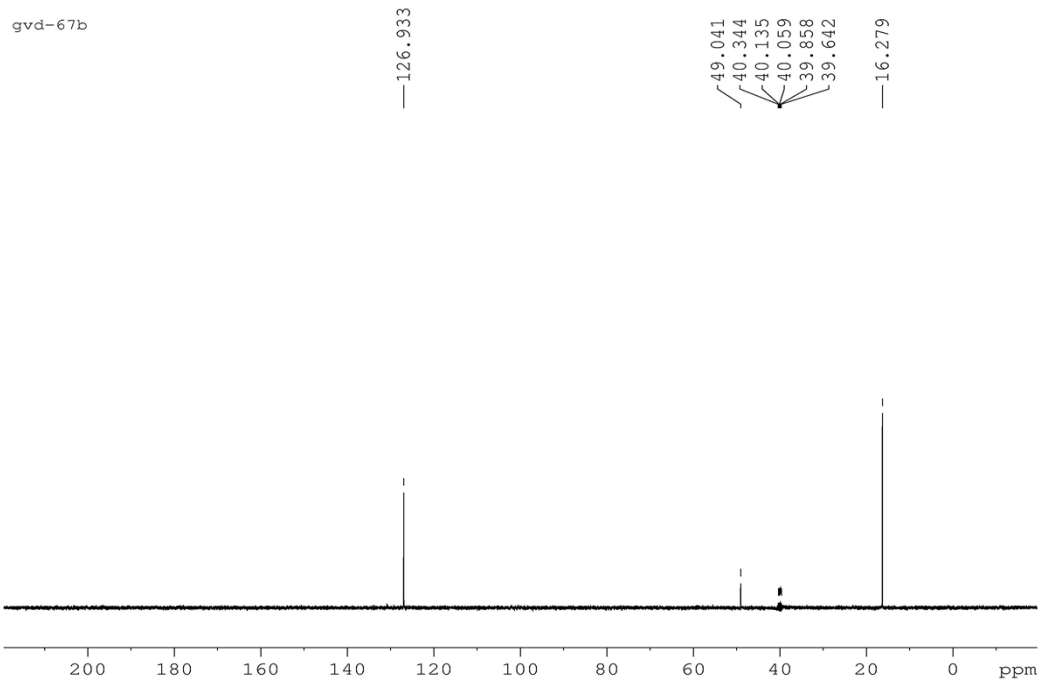
10a. ^{1}H NMR



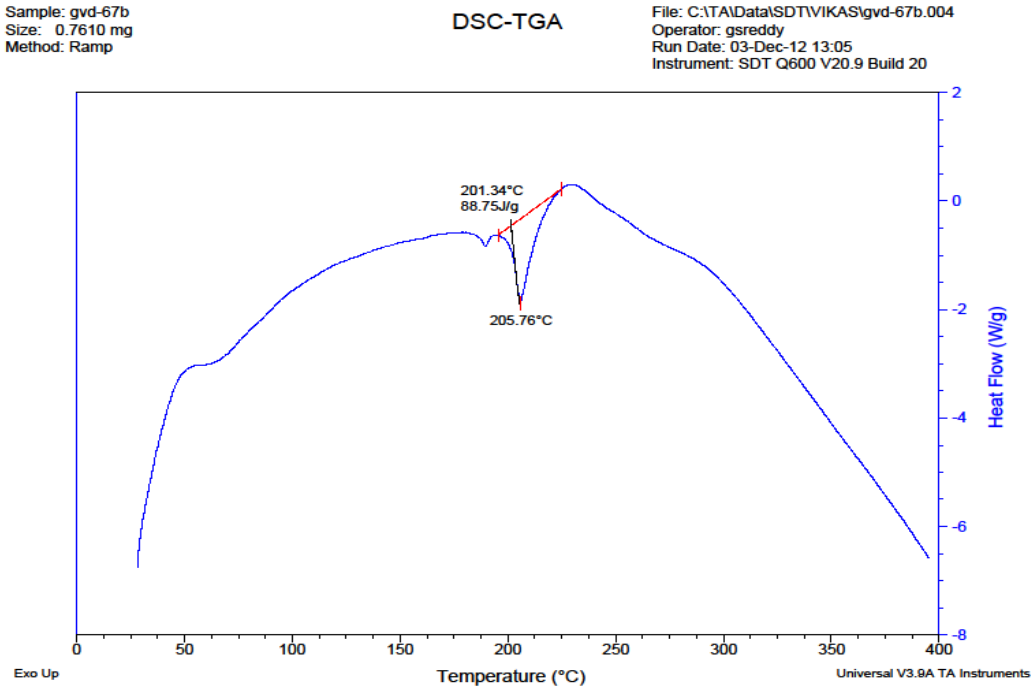
10b. ^{13}C NMR



10c. DEPT

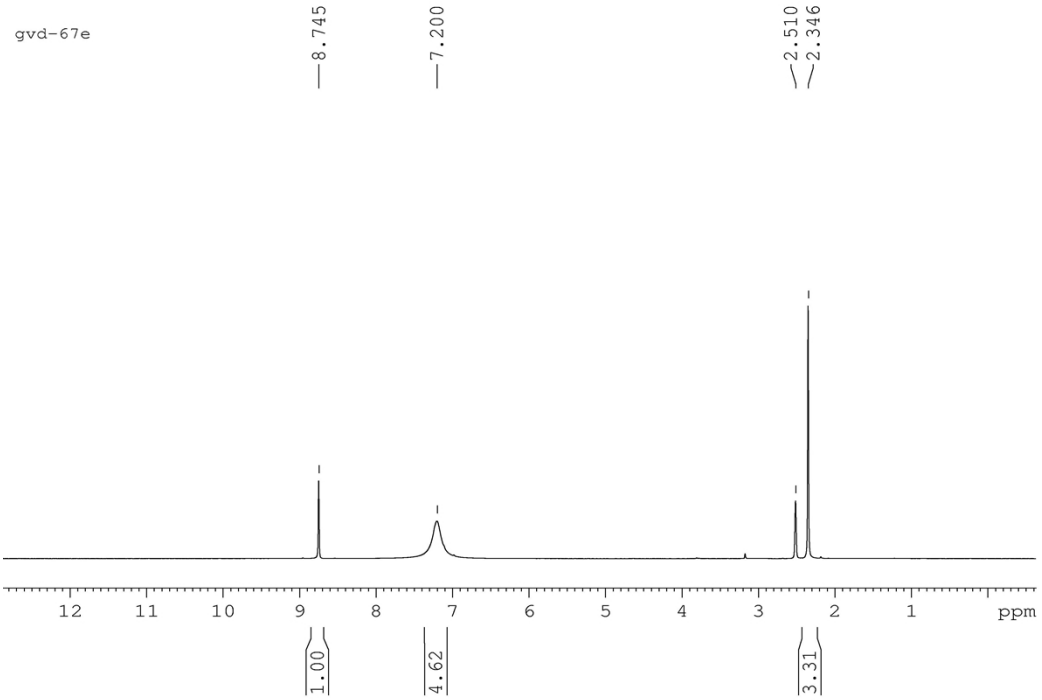


10d. TG-DTA

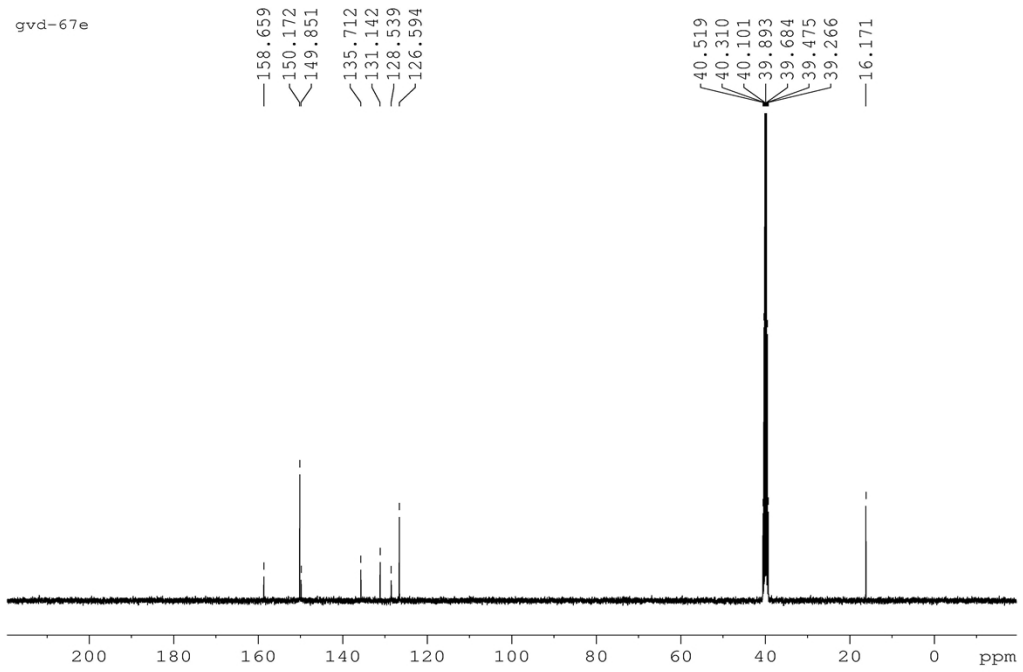


11. **3,4-Diamino-1,2,5-oxadiazol-2-ium 3-methyl-2,4,6-trinitrophenolate (2d)**

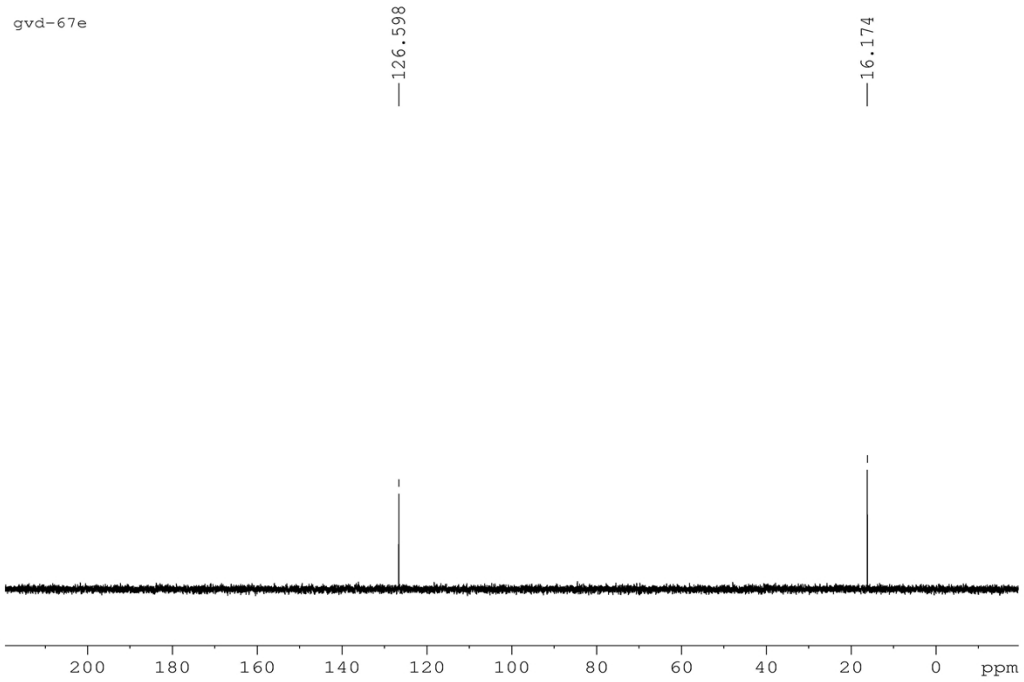
11a. ^{1}H NMR



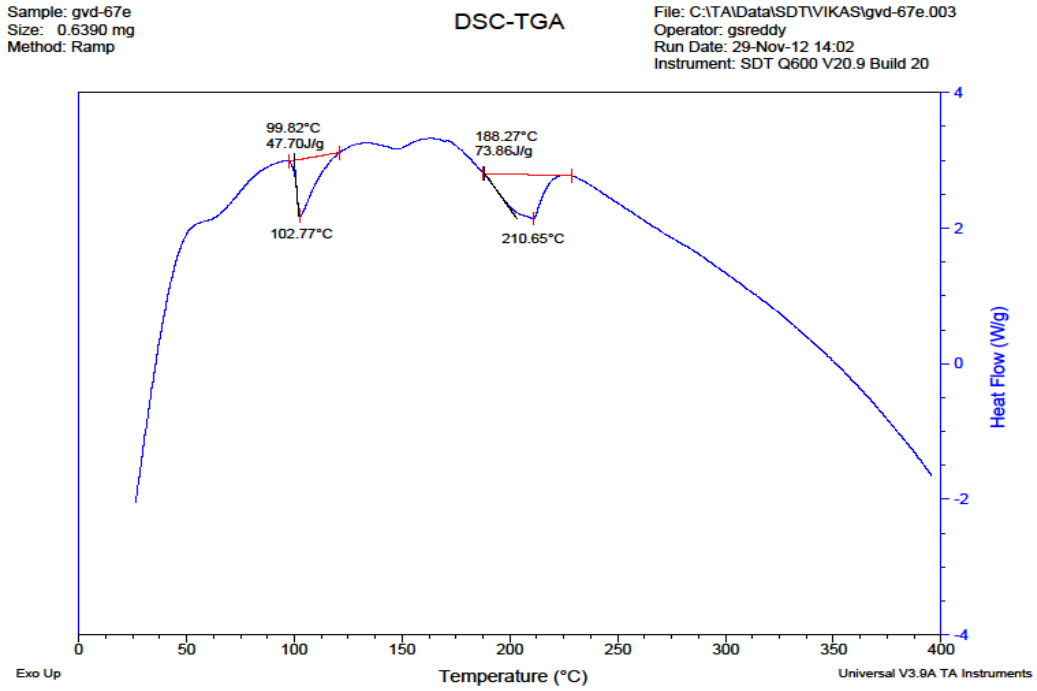
11b. ^{13}C NMR



11c. DEPT

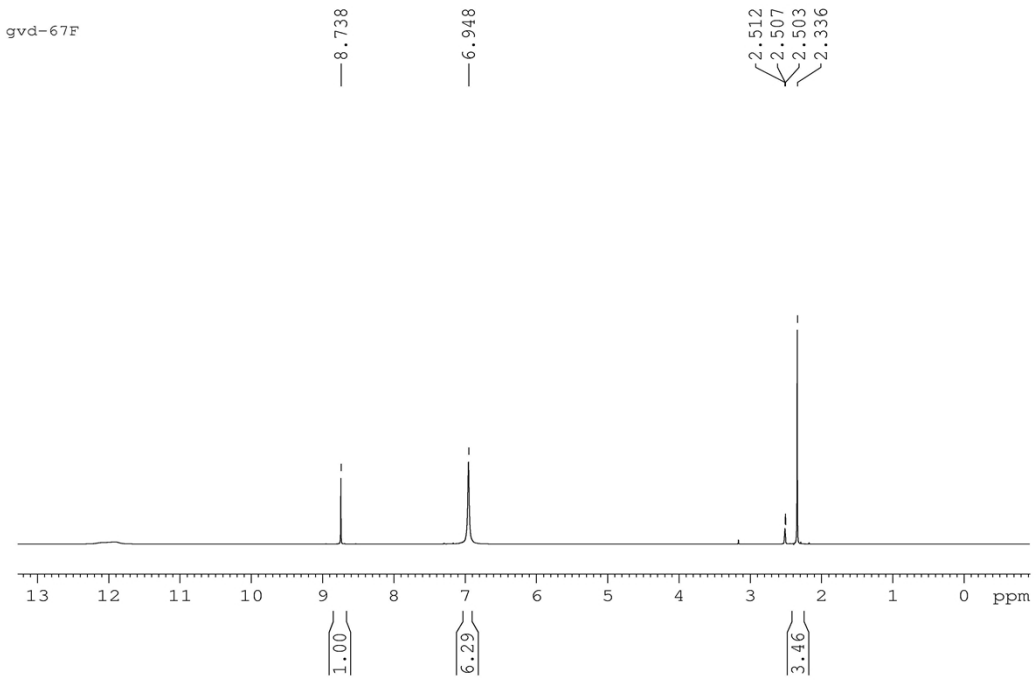


11d. TG-DTA

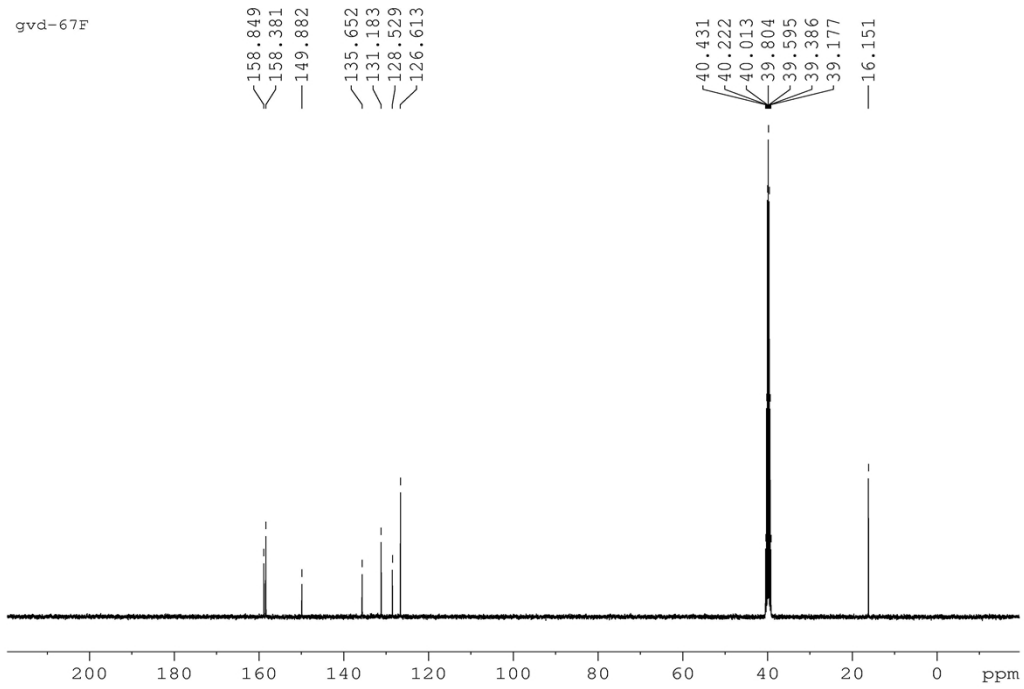


12. **Diaminomethaniminium 3-methyl-2,4,6-trinitrophenolate (2e)**

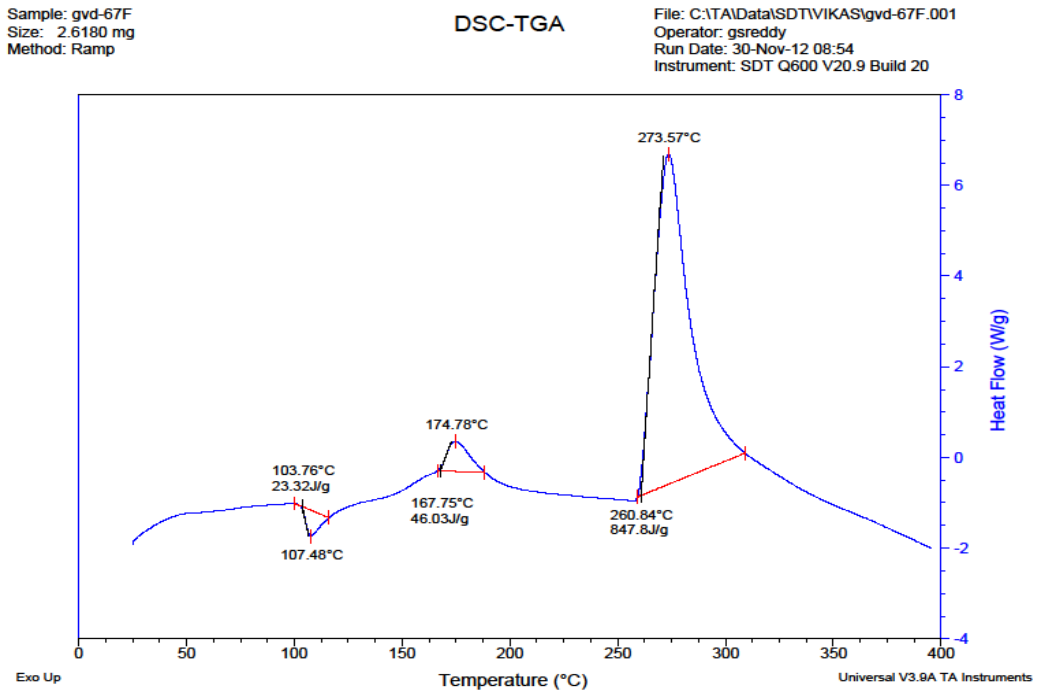
12a. ^{1}H NMR



12b. ^{13}C NMR

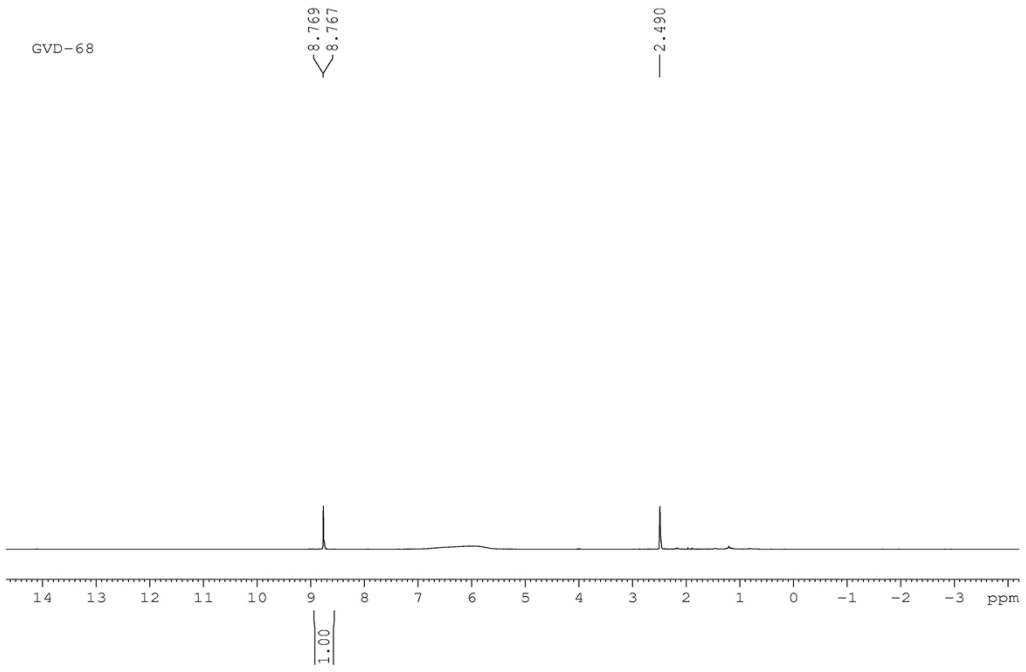


12c. TG-DTA

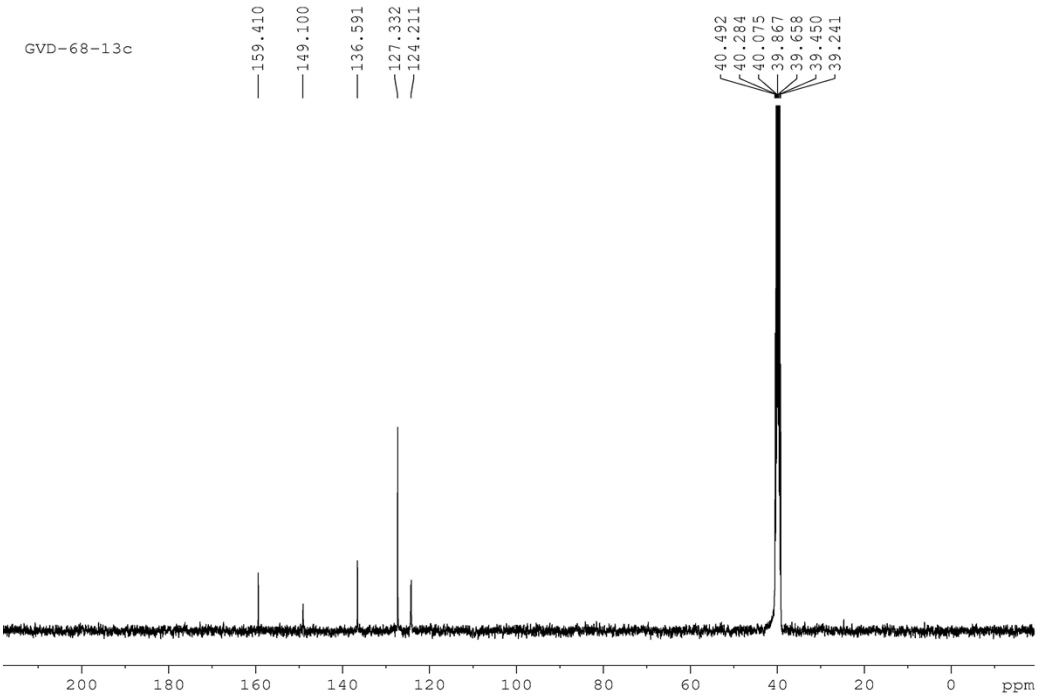


13. **3-Azido-2,4,6-trinitrophenol**

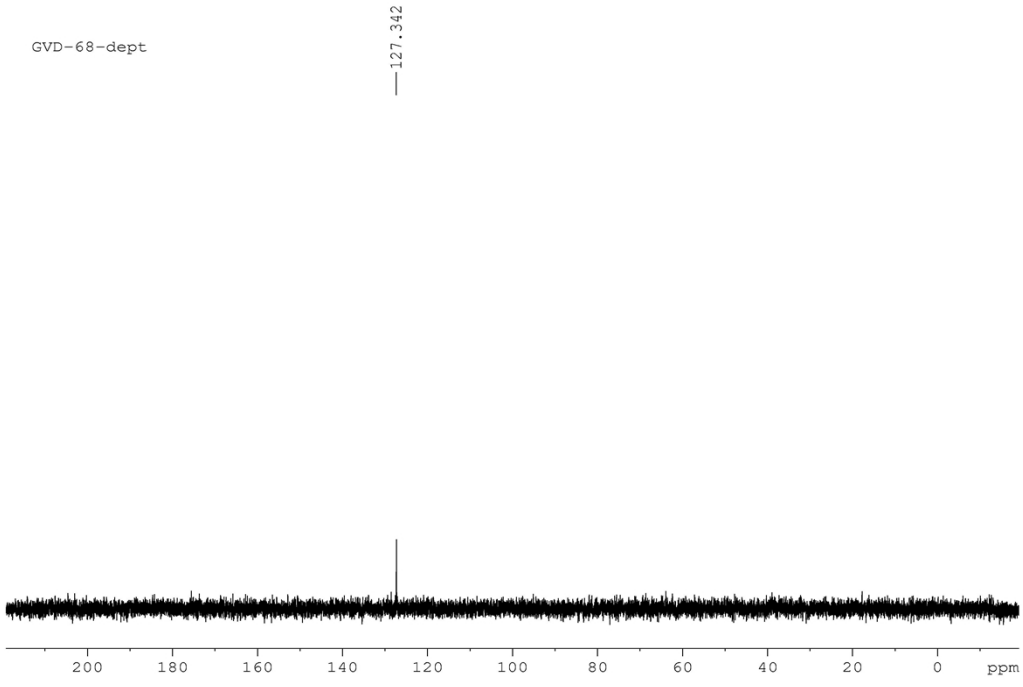
13a. ^{1}H NMR



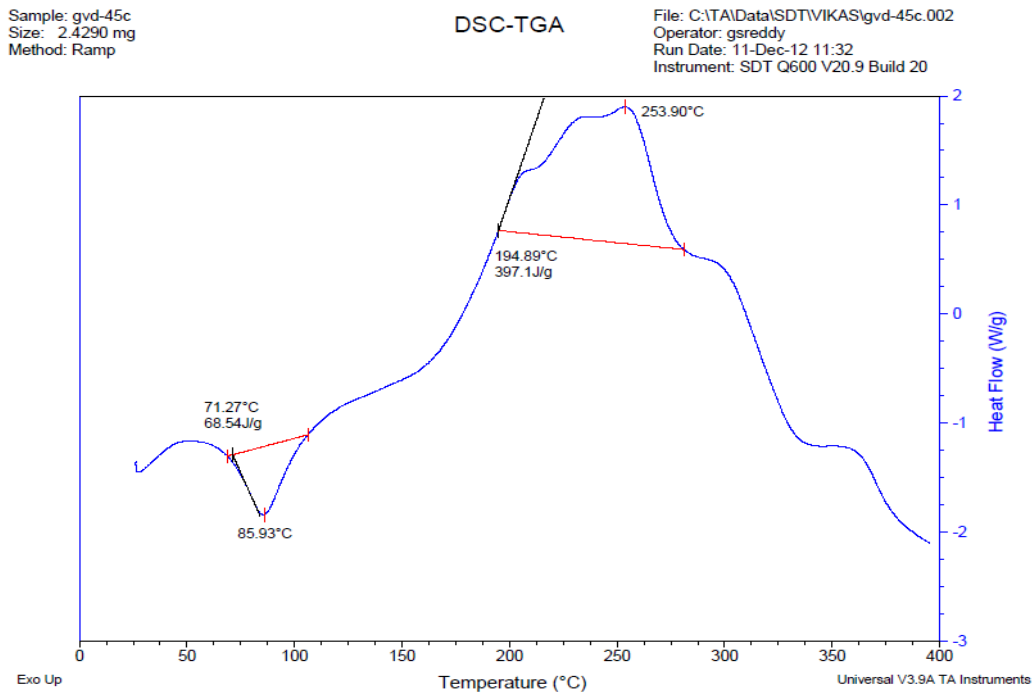
13b. ^{13}C NMR



13c. DEPT

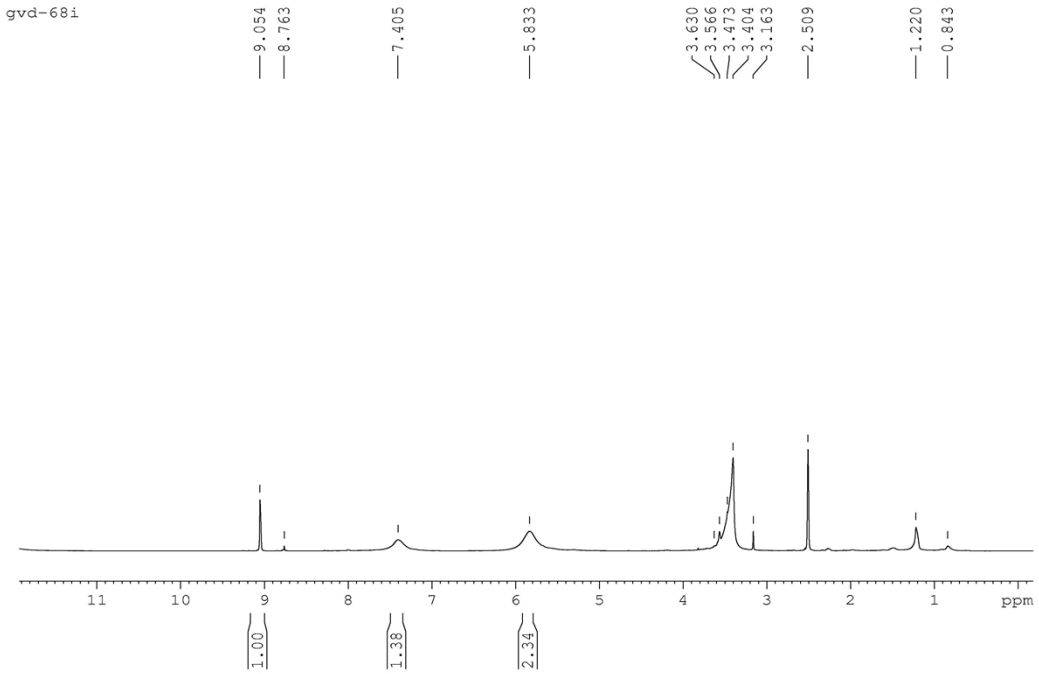


13d. TG-DTA

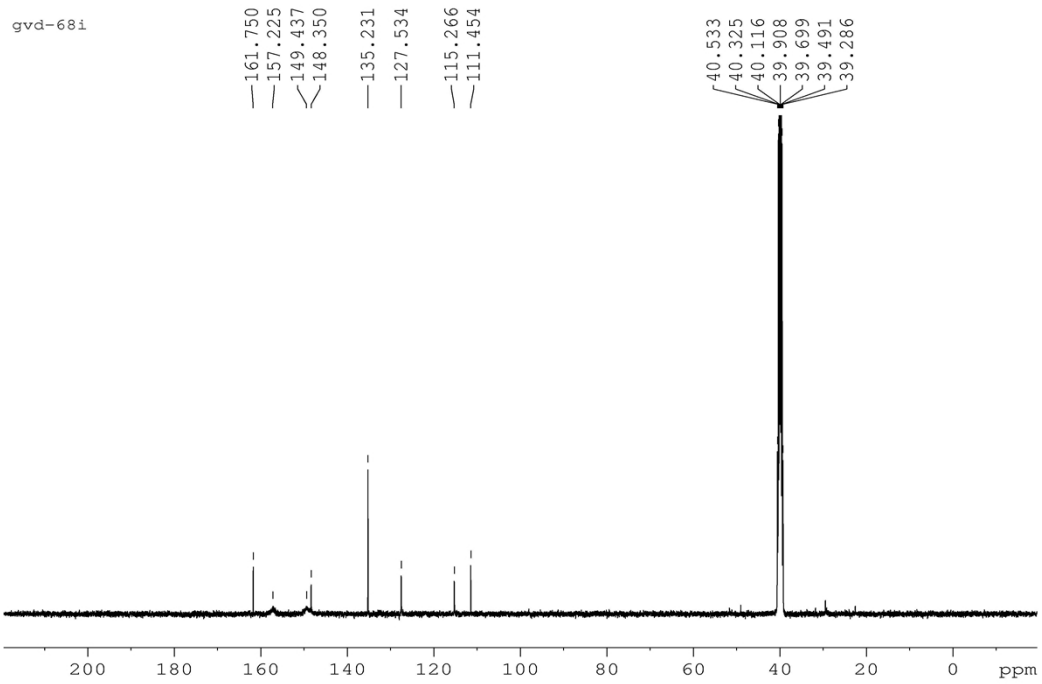


14. **3-Amino-1H-1,2,4-triazol-4-ium 3-azido-2,4,6-trinitrophenolate (3b)**

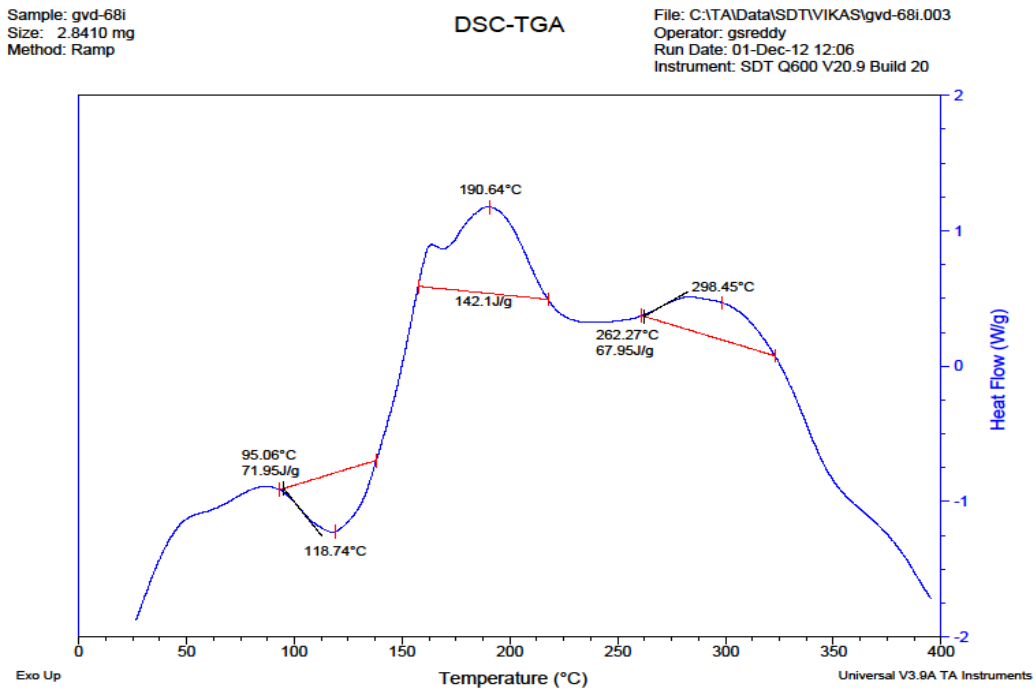
14a. ^{1}H NMR



14b. ^{13}C NMR

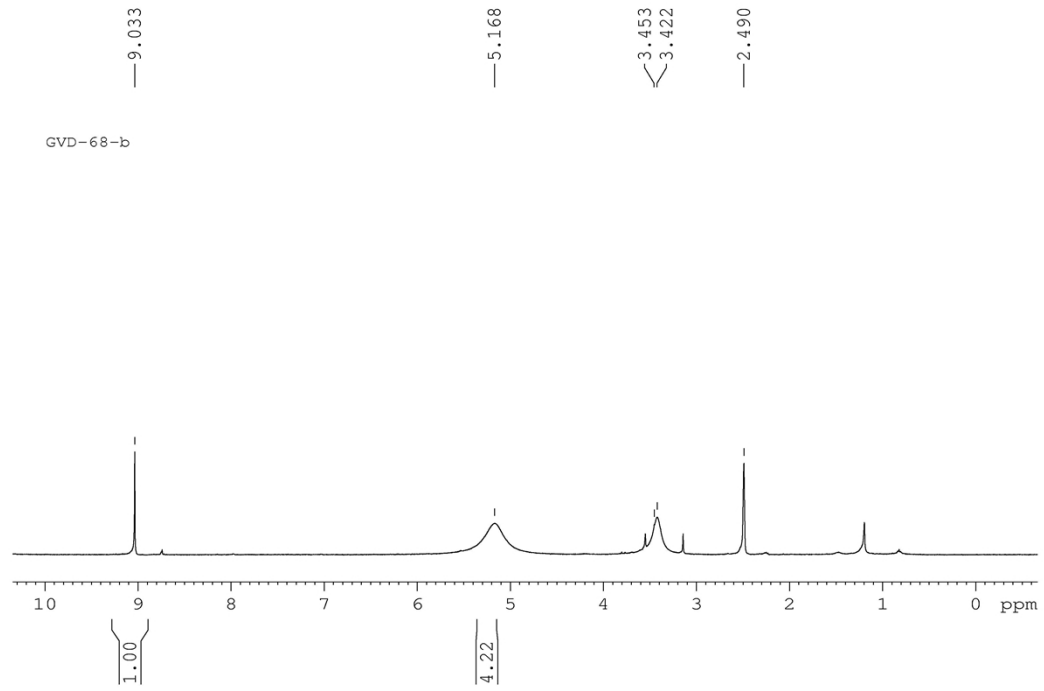


14c. TG-DTA

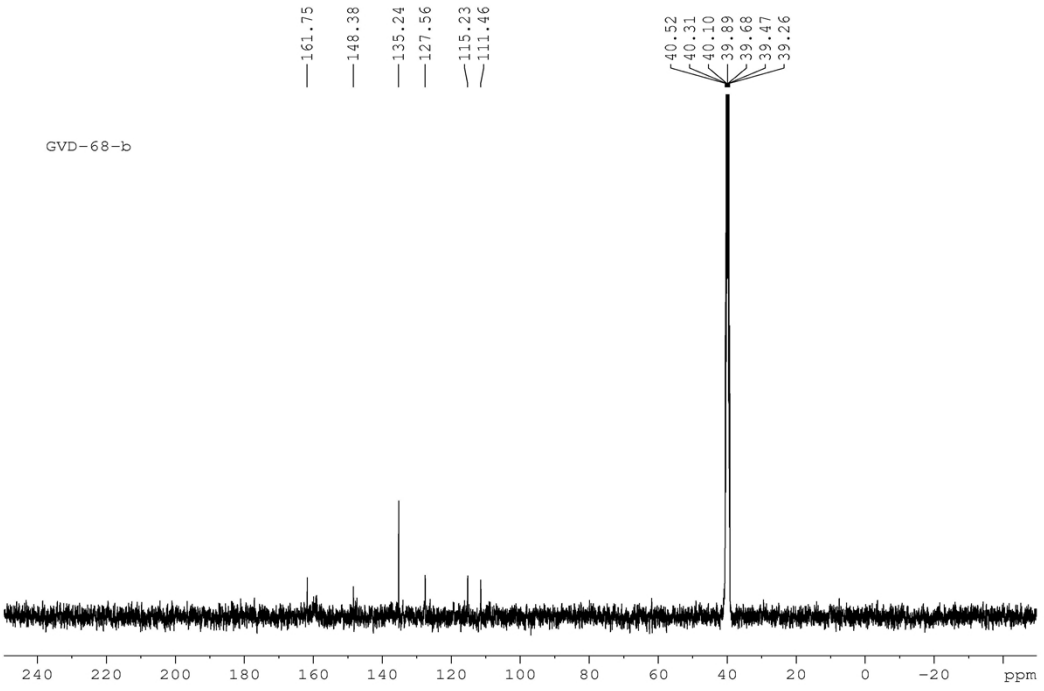


15. **3,5-Diamino-1H-1,2,4-triazol-4-ium 3-azido-2,4,6-trinitrophenolate (3c)**

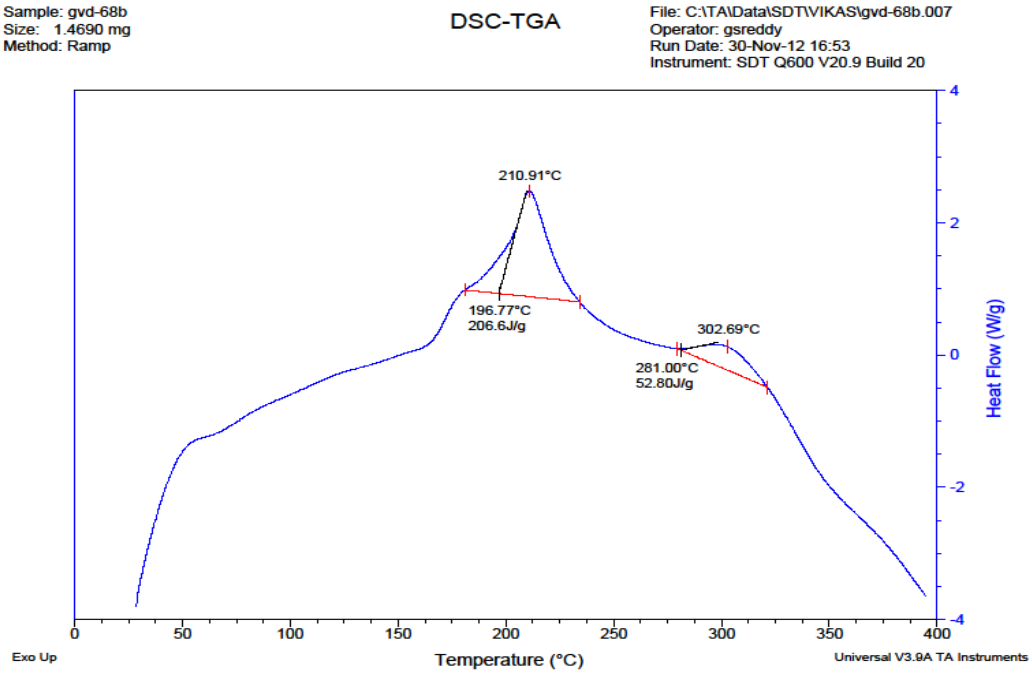
15a. ^{1}H NMR



15b. ^{13}C NMR

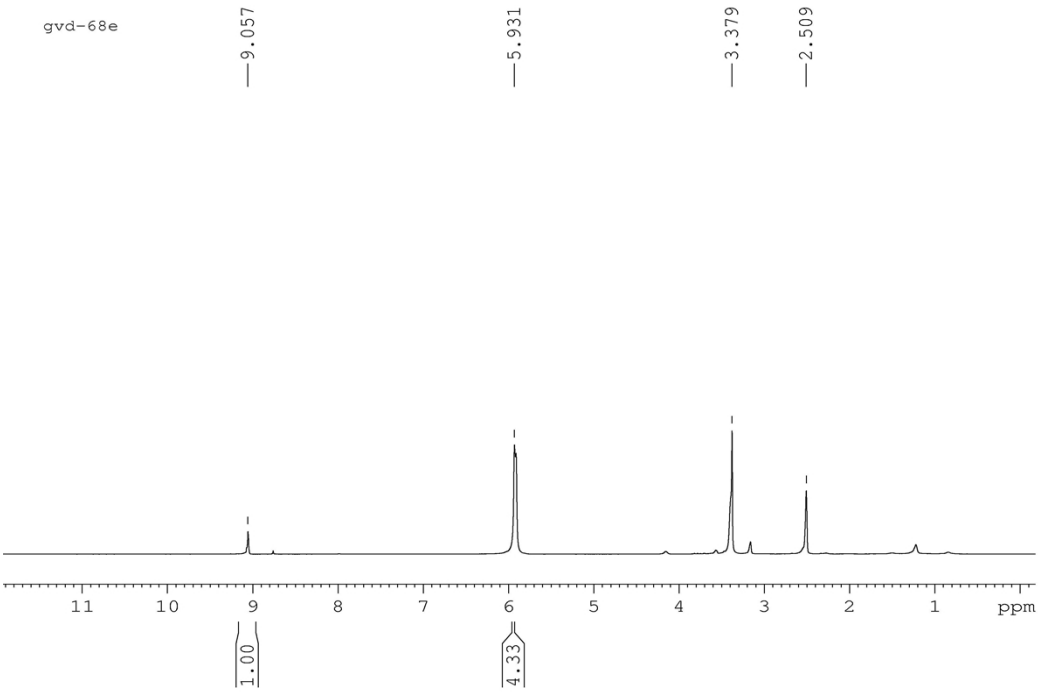


15c. TG-DTA

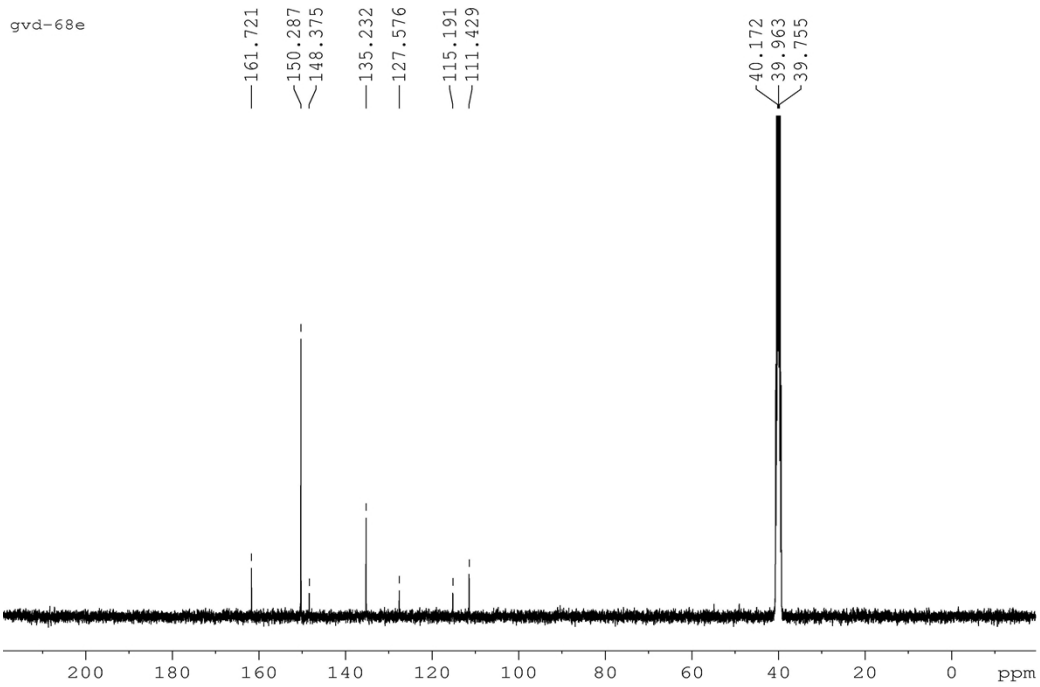


16. **3,4-Diamino-1,2,5-oxadiazol-2-ium 3-azido-2,4,6-trinitrophenolate (3d)**

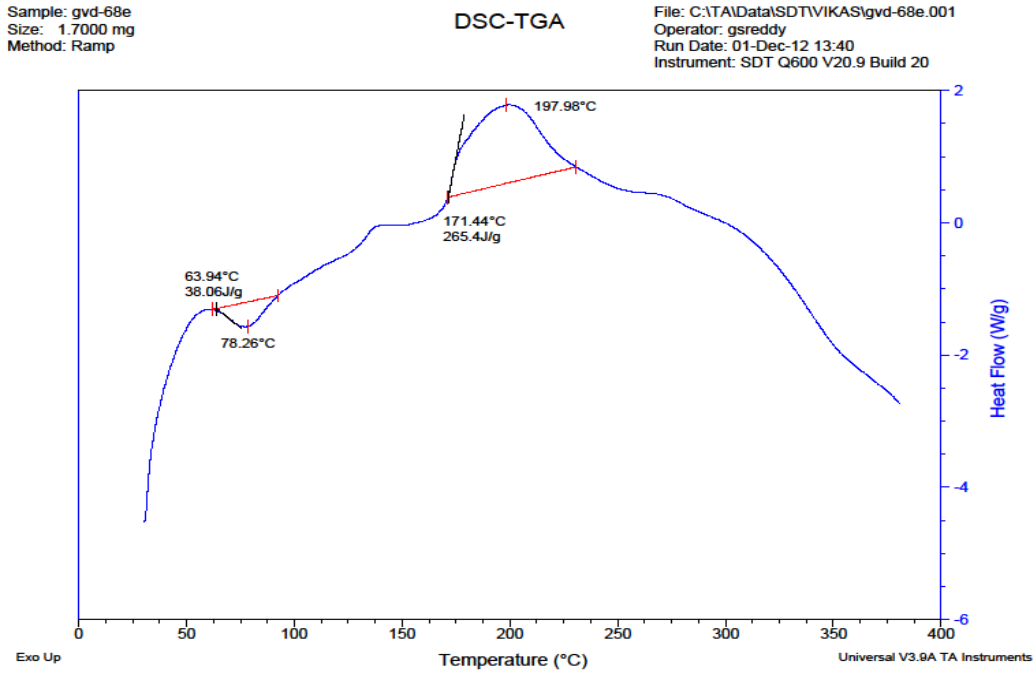
16a. ^{1}H NMR



16b. ^{13}C NMR

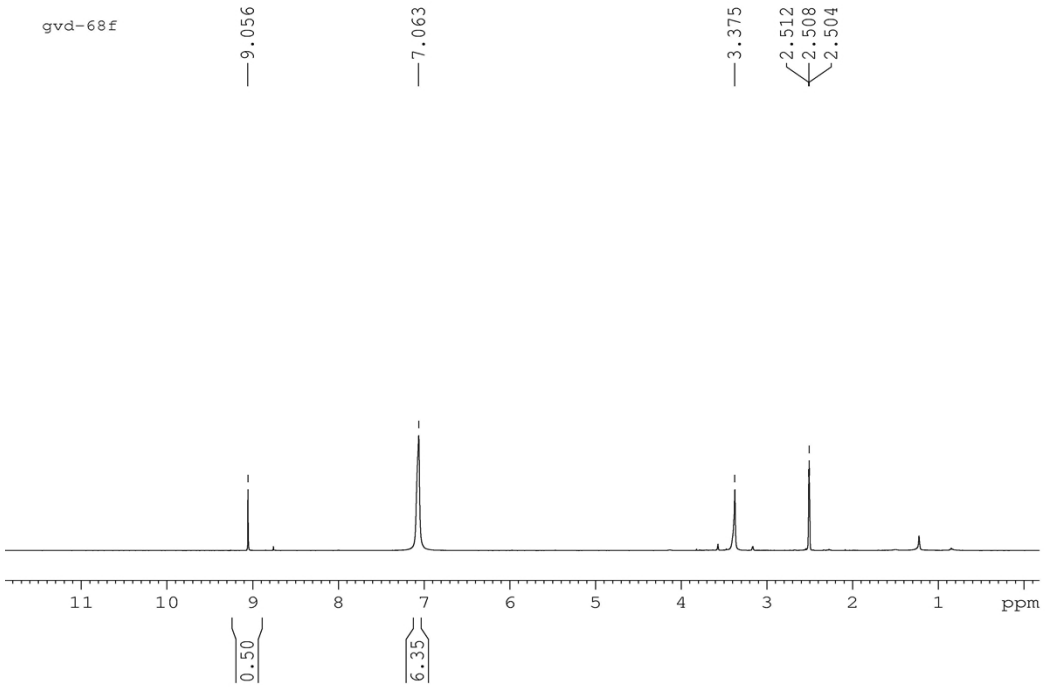


16c. TG-DTA

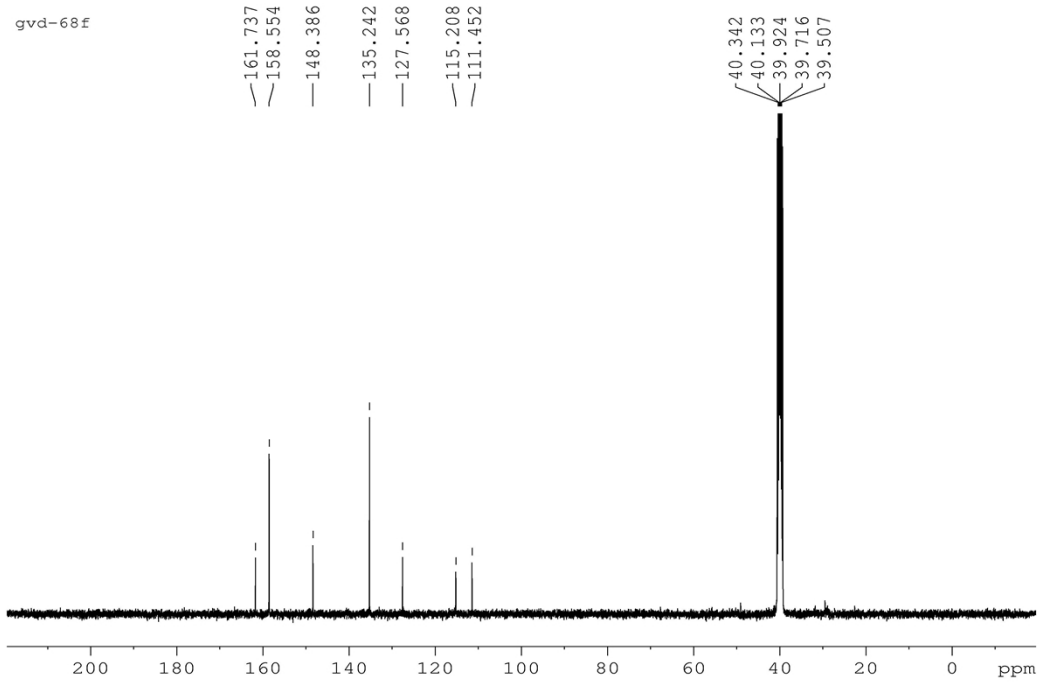


17. **Diaminomethaniminium 3-azido-2,4,6-trinitrophenolate (3e)**

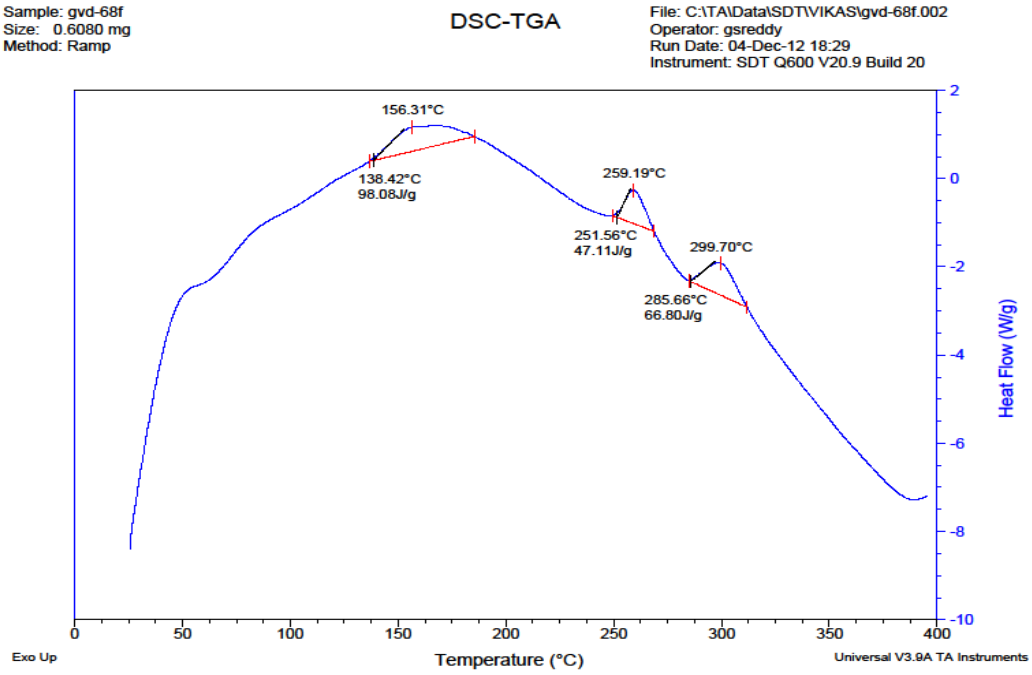
17a. ^{1}H NMR



17b. ^{13}C NMR

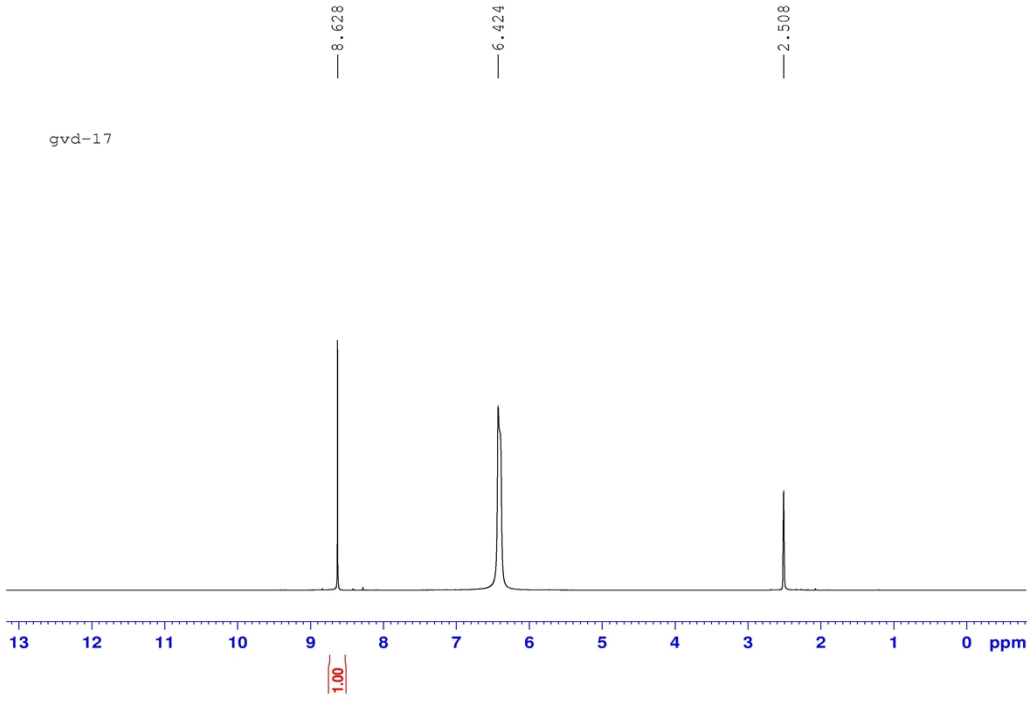


17c. TG-DTA

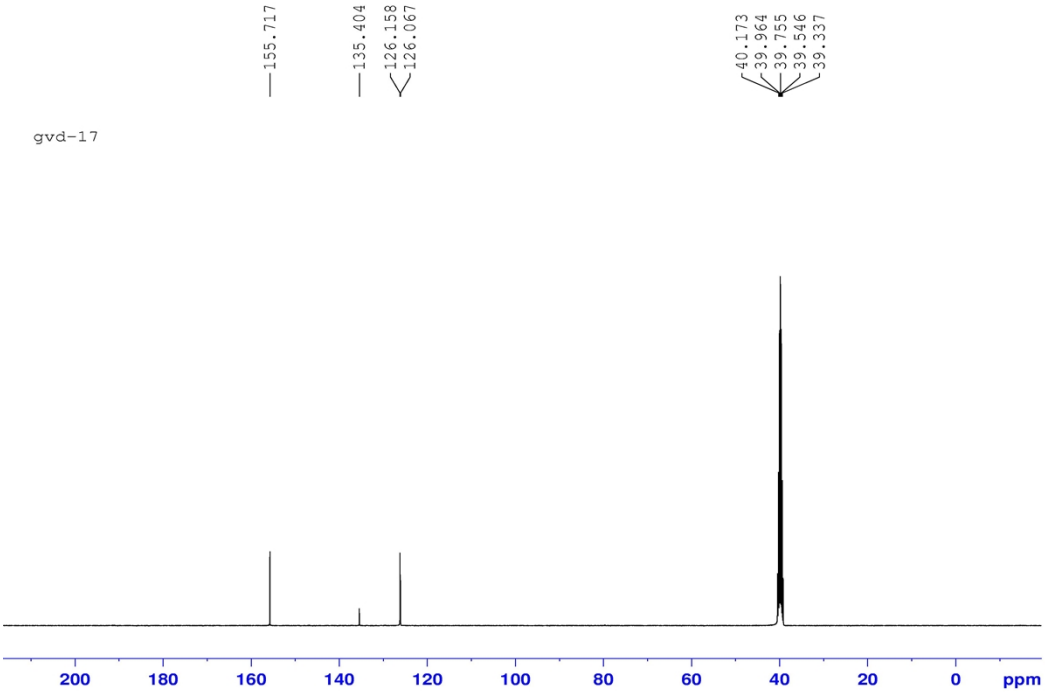


18. **Styphnic acid**

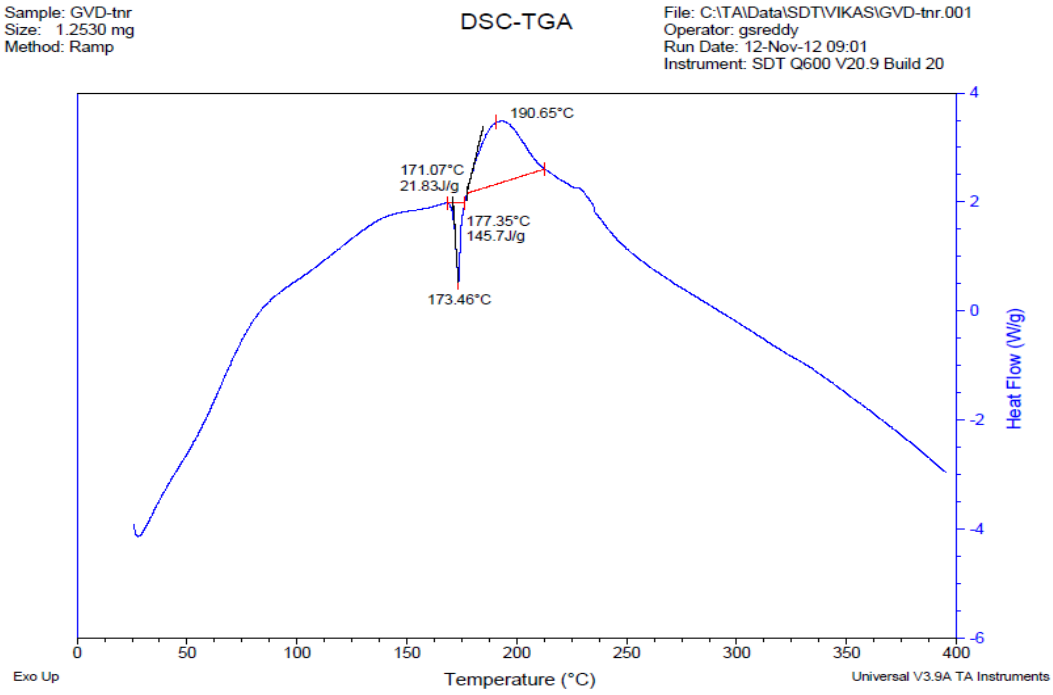
18a. ^{1}H NMR



18b. ^{13}C NMR

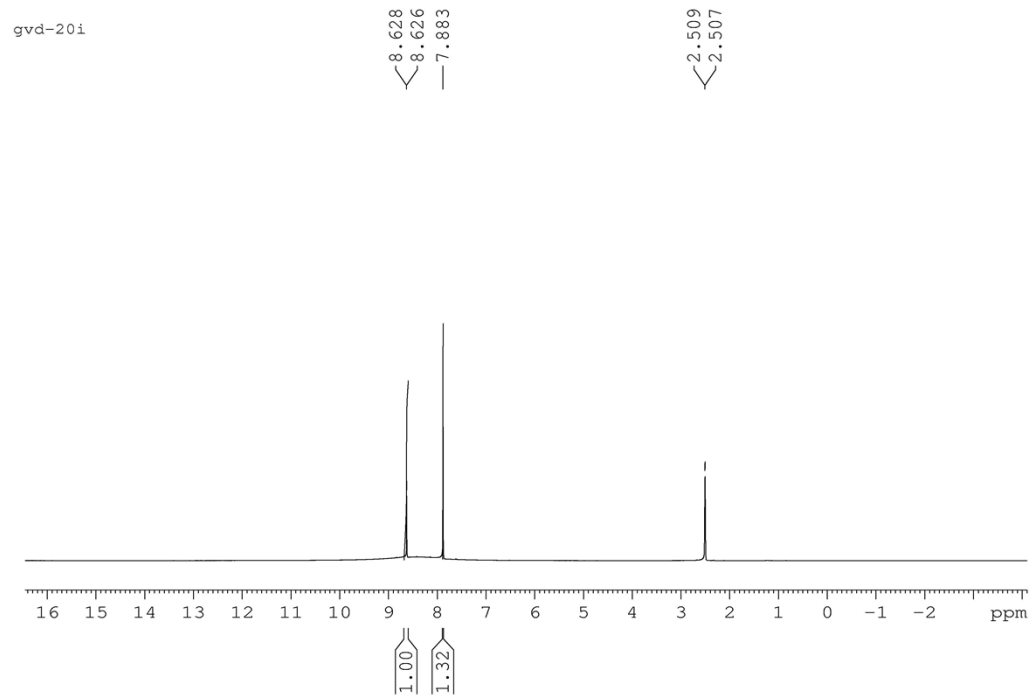


18c. TG-DTA

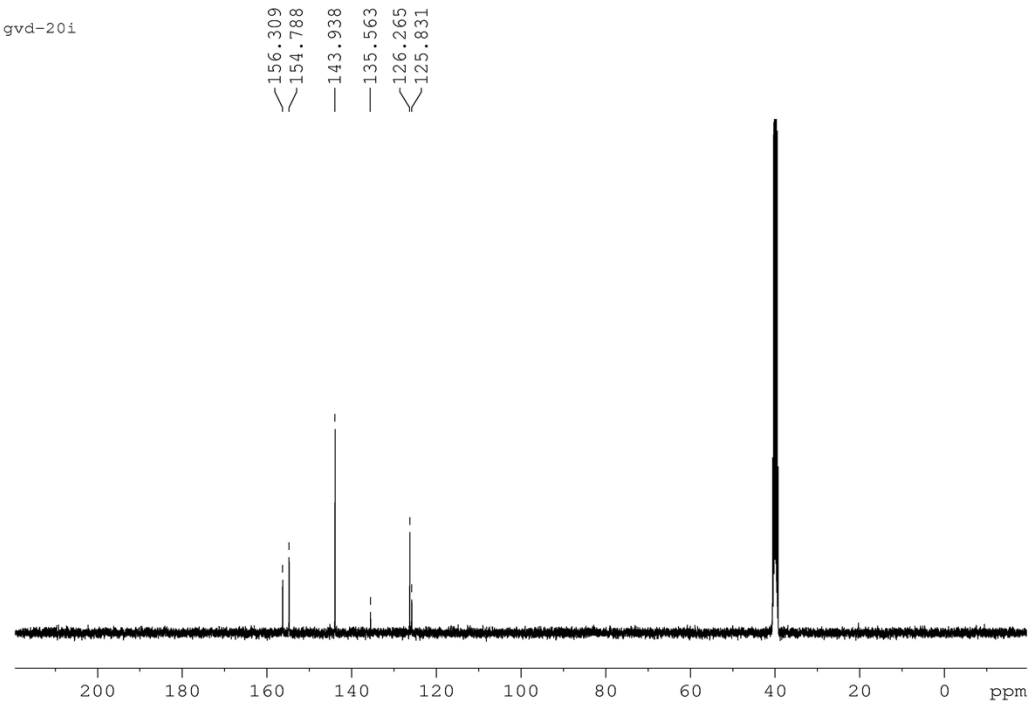


19. **Bis(3-amino-1H-1,2,4-triazol-4-ium) 2,4,6-trinitrobenzene-1,3-diolate (4b)**

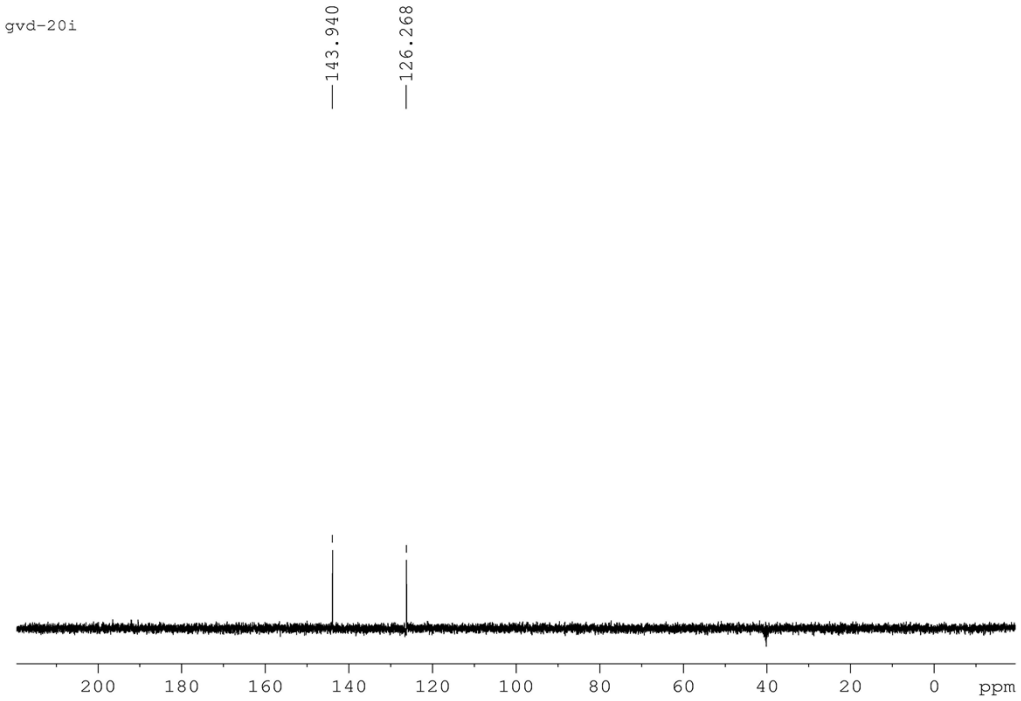
19a. ^{1}H NMR



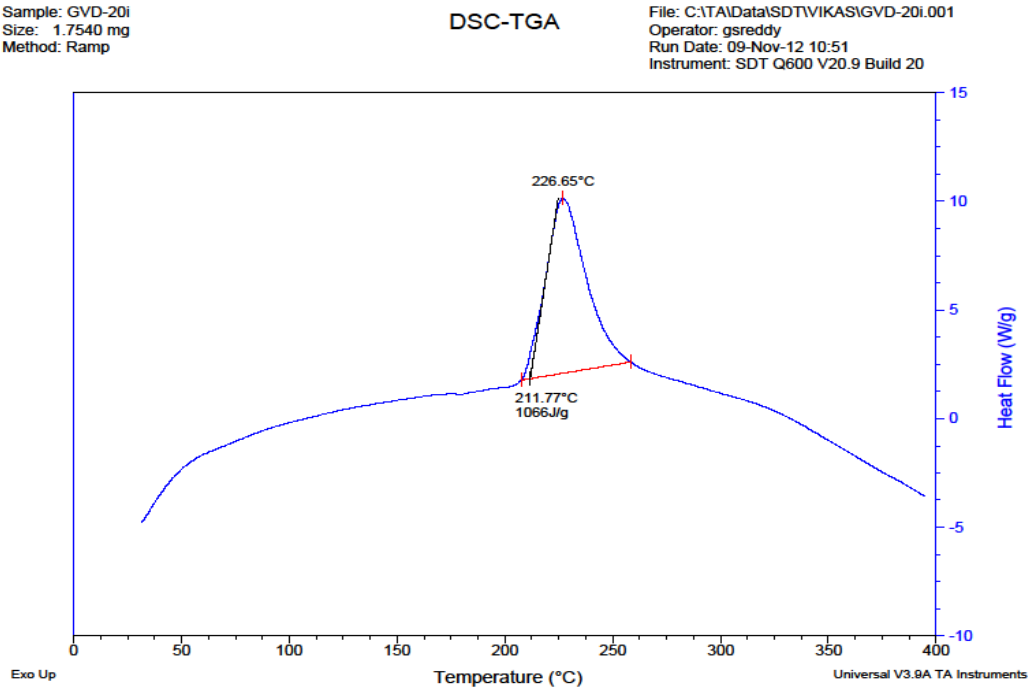
19b. ^{13}C NMR



19c. DEPT

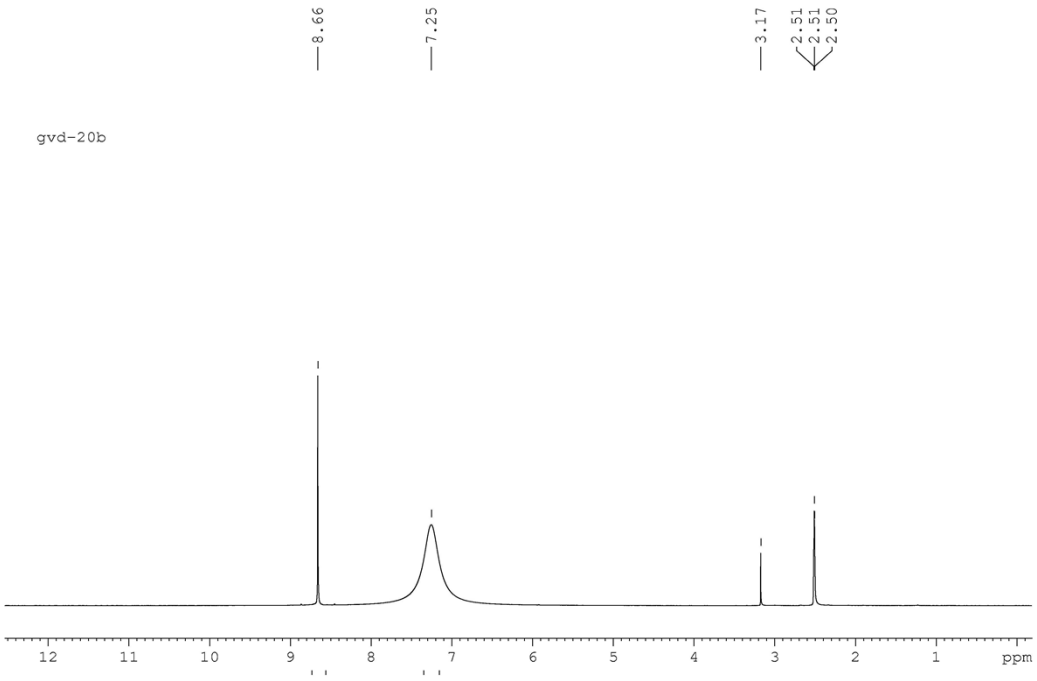


19d. TG-DTA

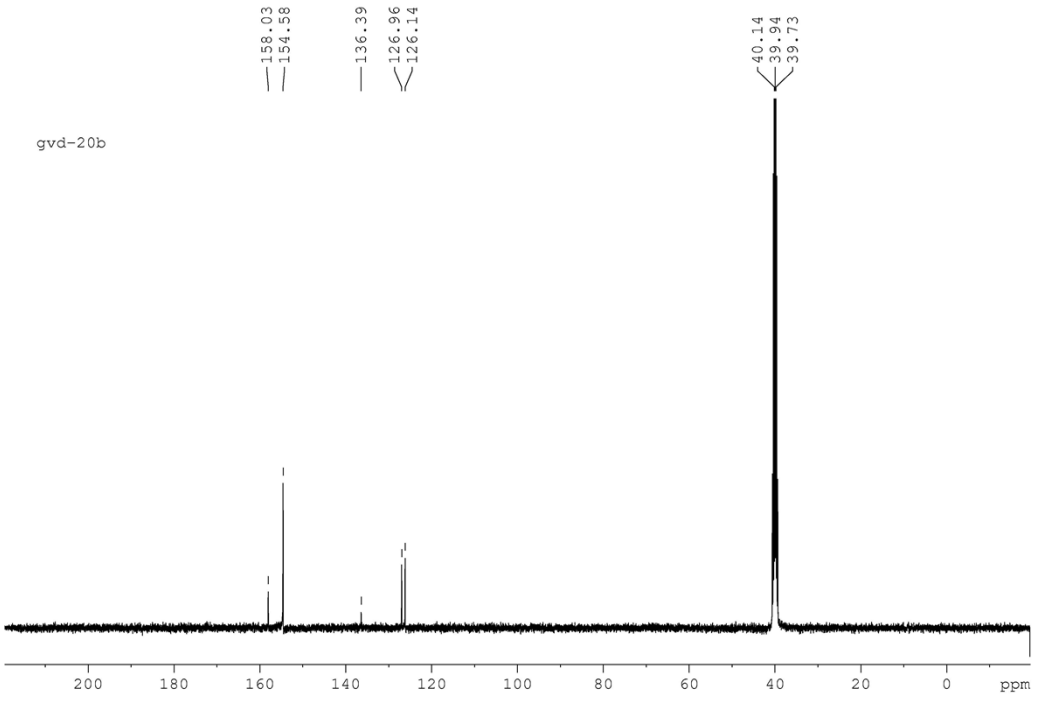


20. **Bis(3,5-diamino-1H-1,2,4-triazol-4-ium) 2,4,6-trinitrobenzene-1,3-diolate (4c)**

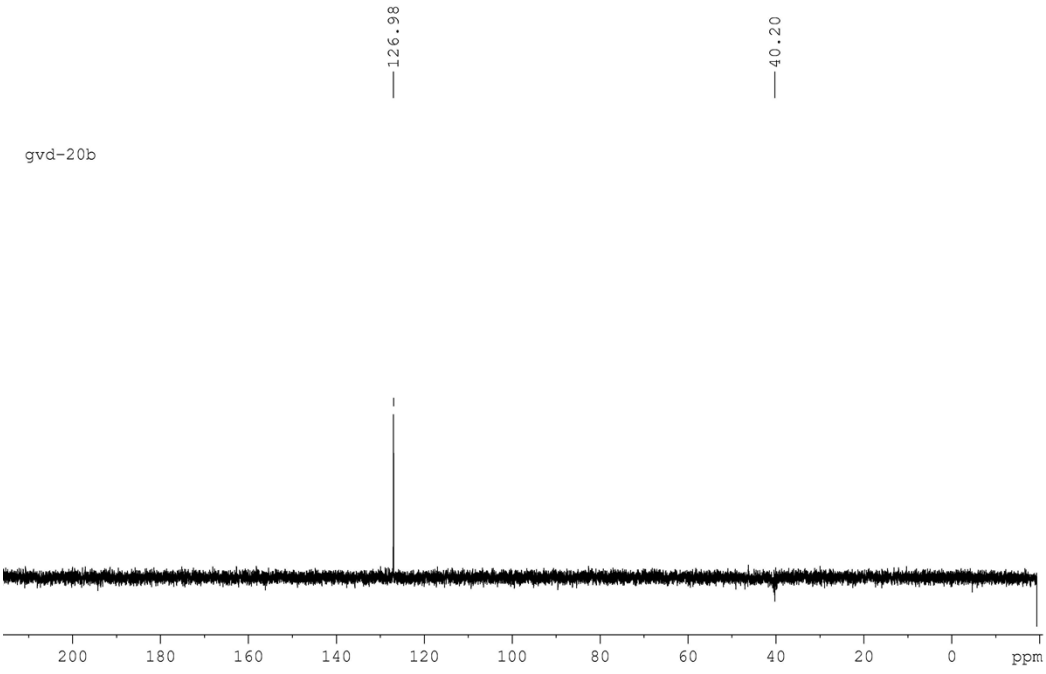
20a. ^{1}H NMR



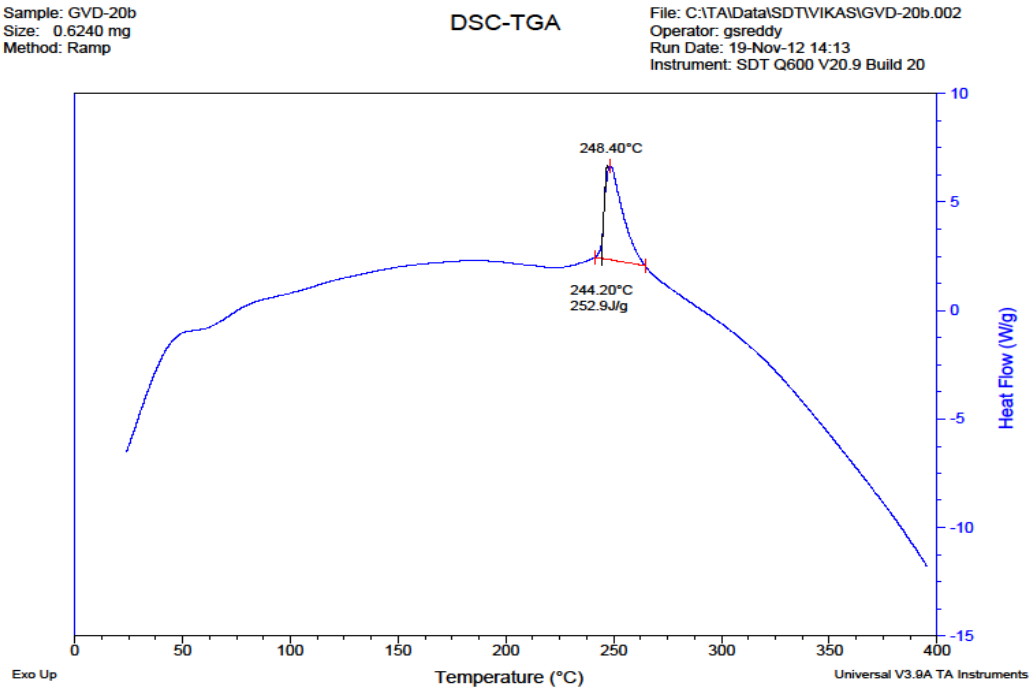
20b. ^{13}C NMR



20c. DEPT

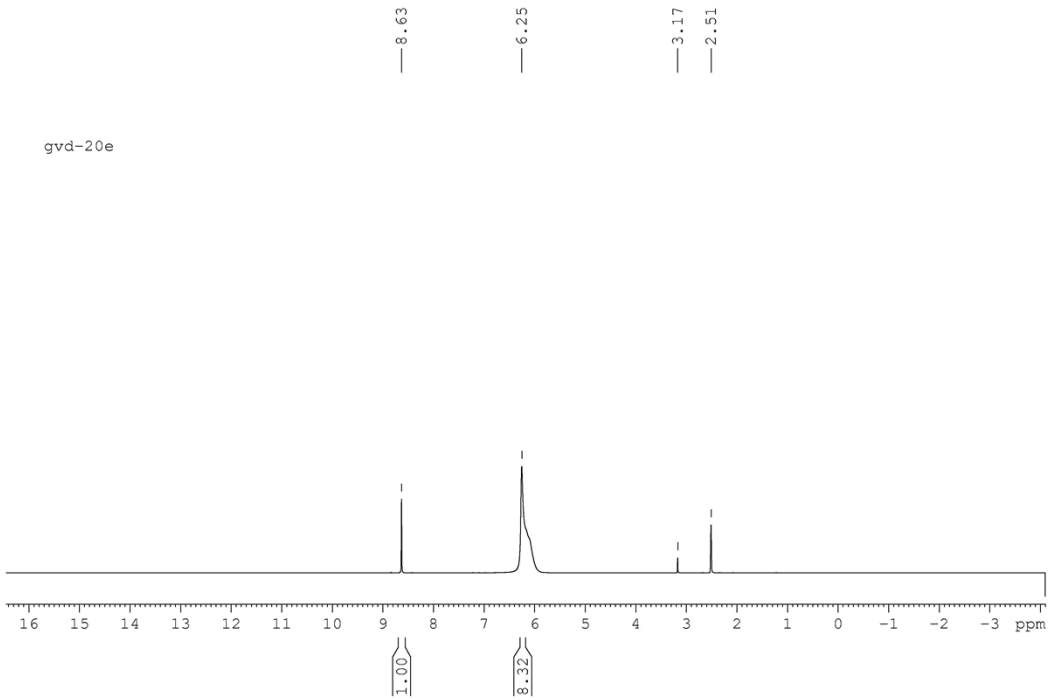


20d. TG-DTA

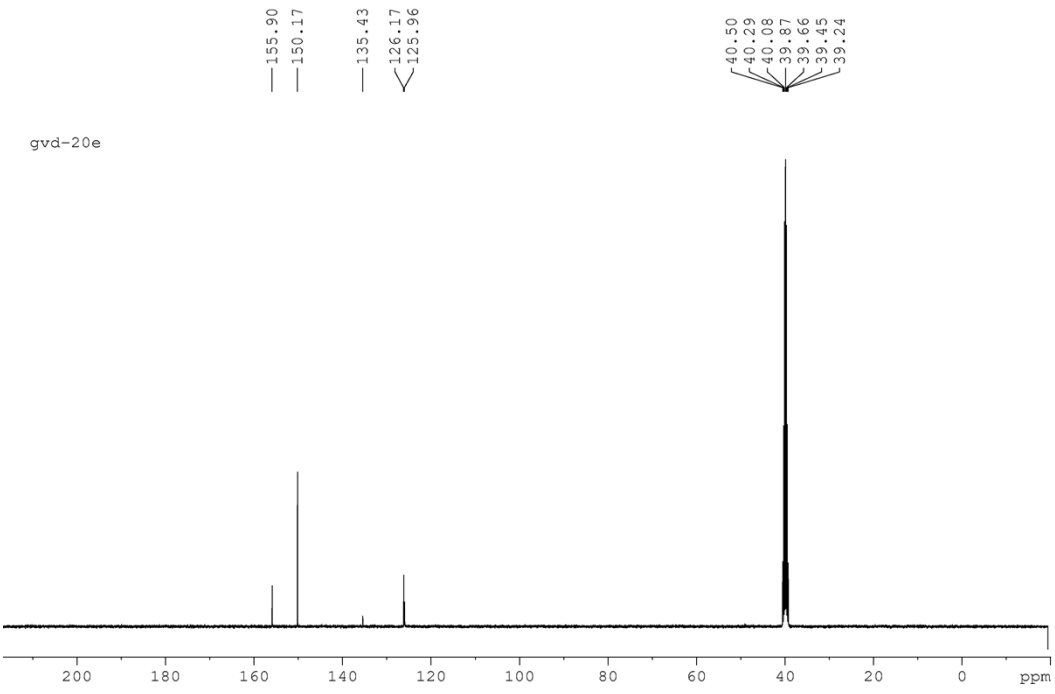


21. **Bis(3,4-diamino-1,2,5-oxadiazol-2-ium) 2,4,6-trinitrobenzene-1,3-diolate (4d)**

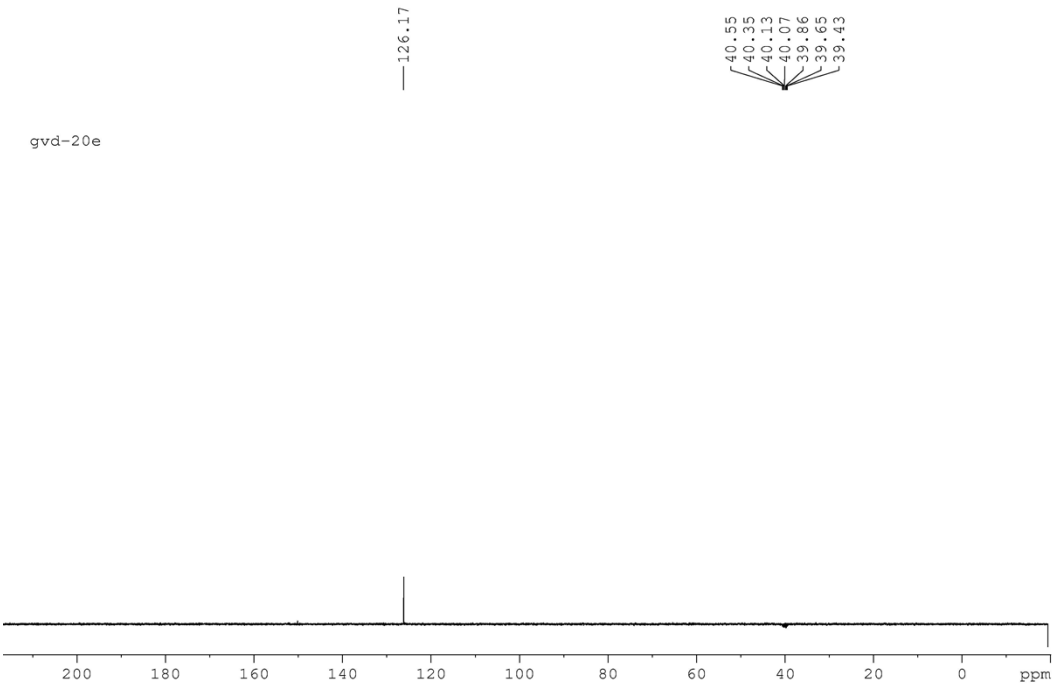
21a. ^{1}H NMR



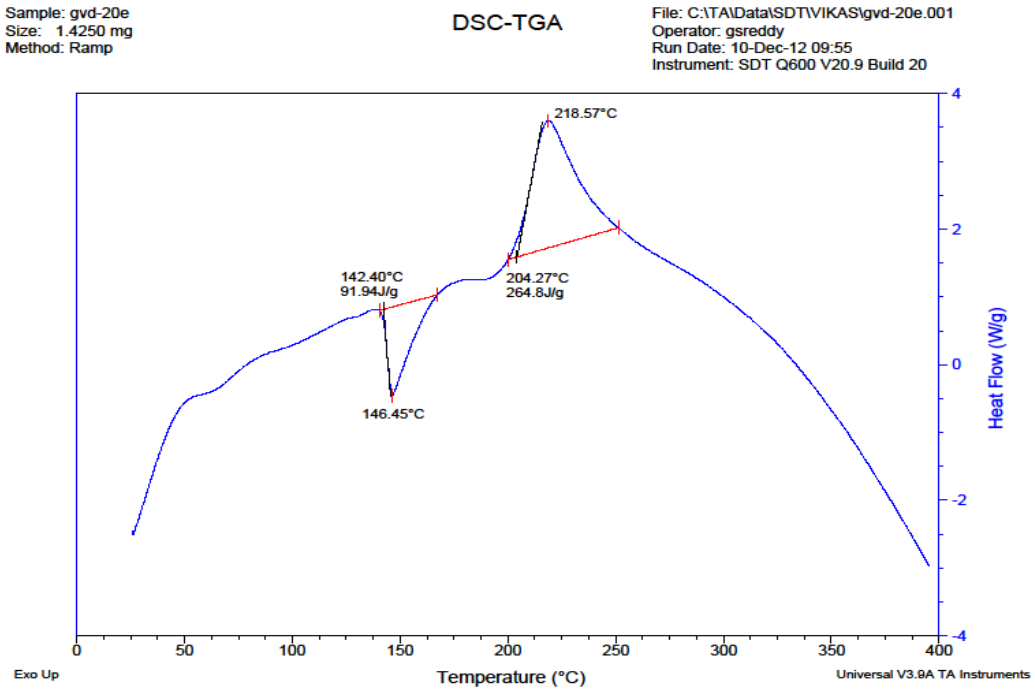
21b. ^{13}C NMR



21c. DEPT

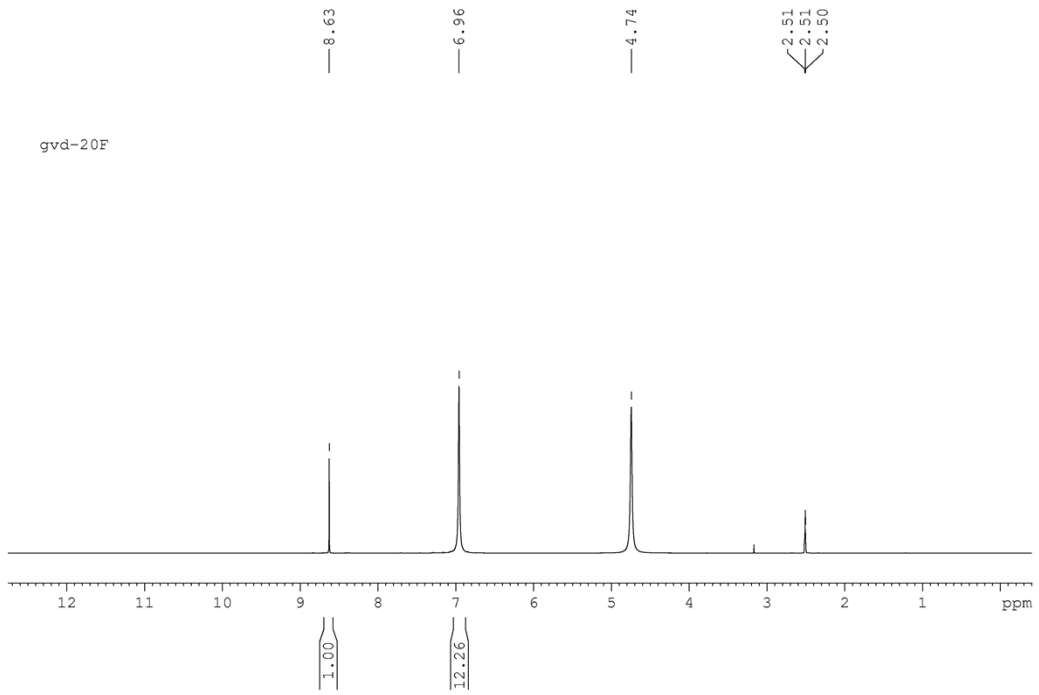


21d. TG-DTA

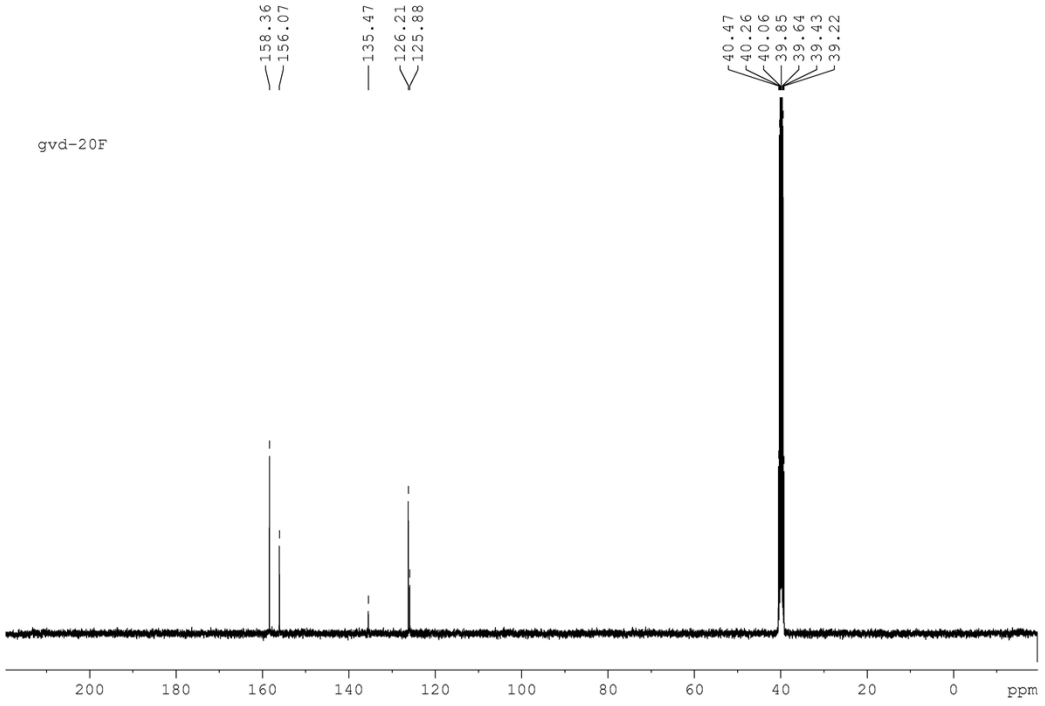


22. **Bis(diaminomethaniminium) 2,4,6-trinitrobenzene-1,3-diolate (4e)**

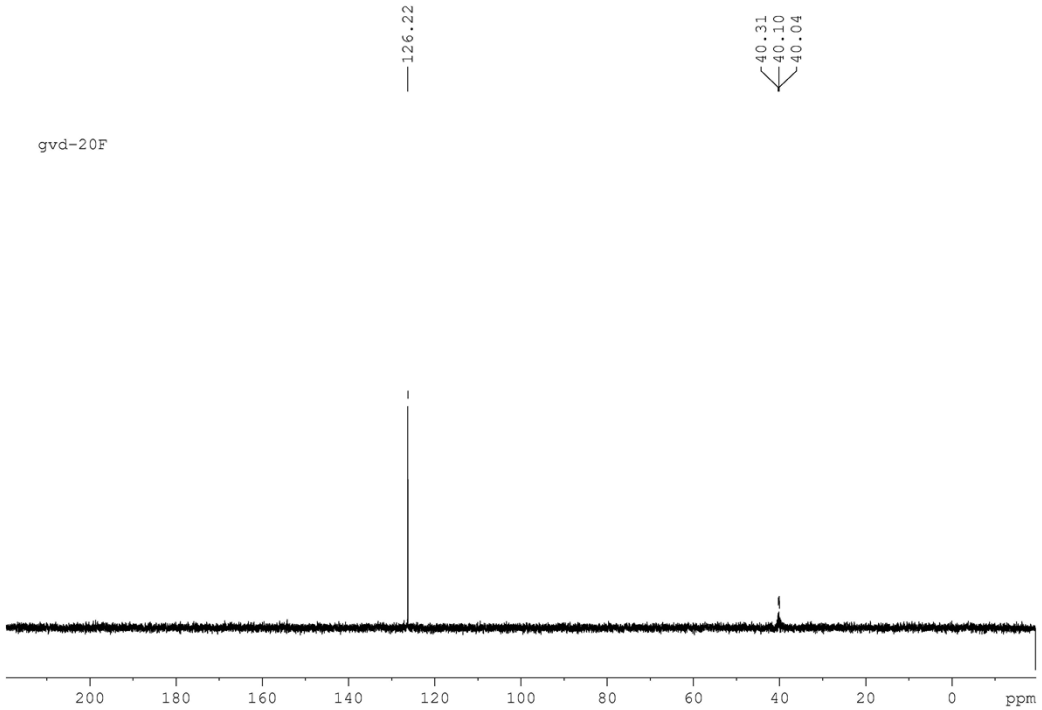
22a. ^{1}H NMR



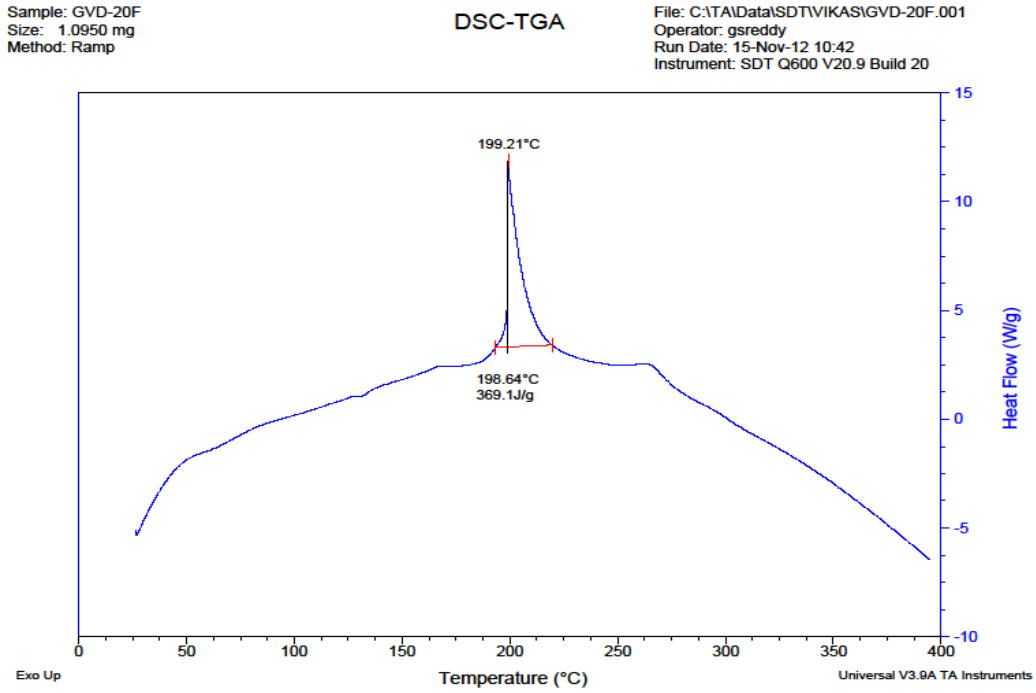
22b. ^{13}C NMR



22c. DEPT

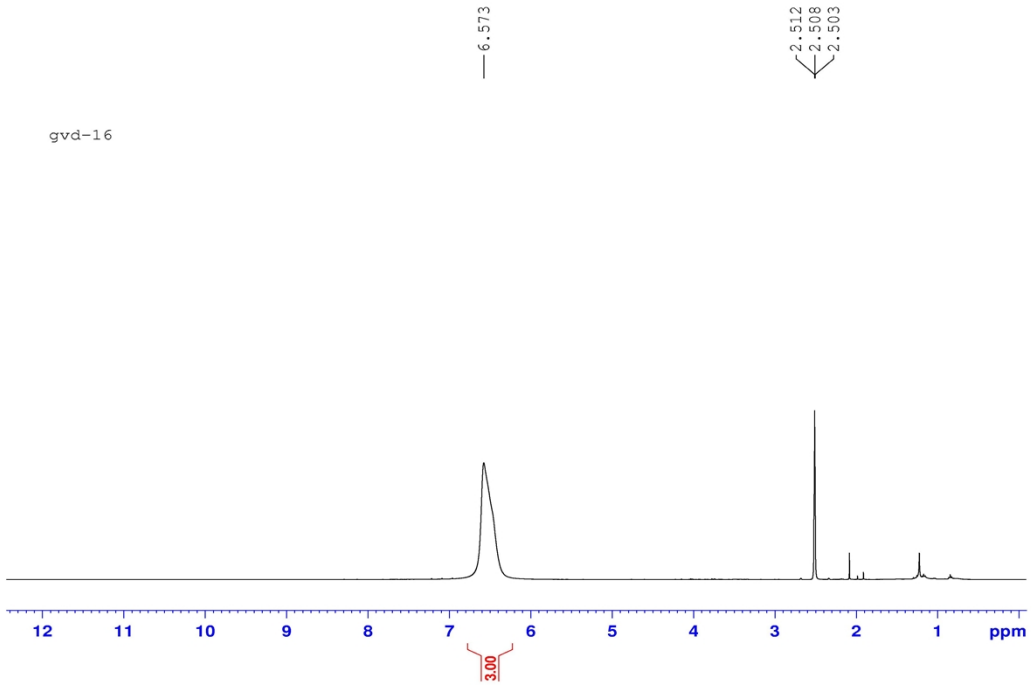


22d. TG-DTA

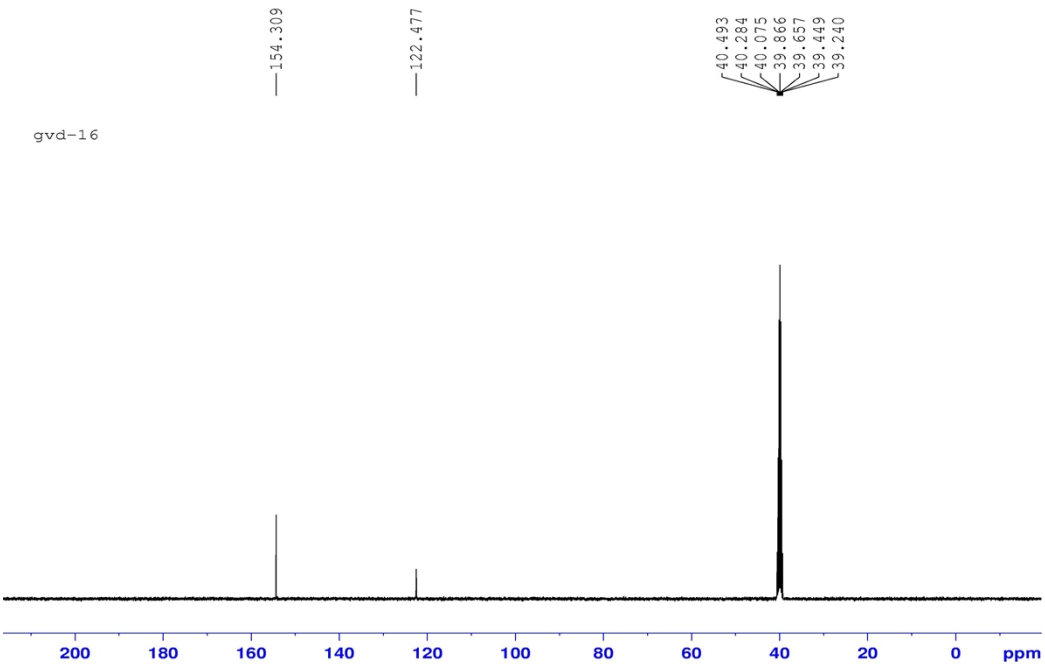


23. **2,4,6-Trinitro-1,3,5-benzenetriol**

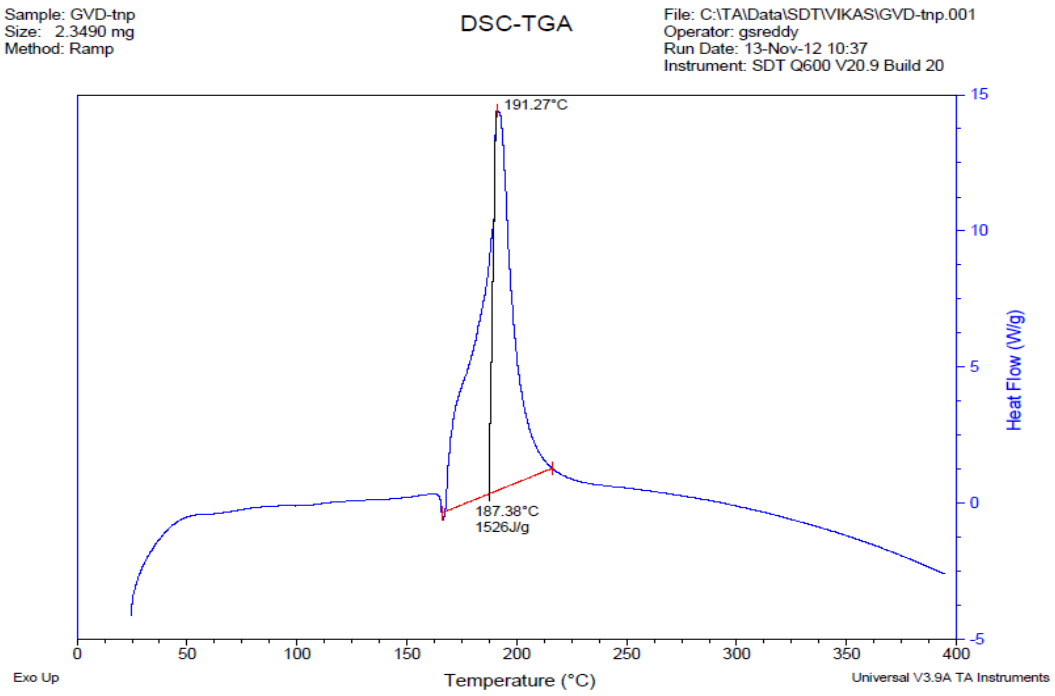
23a. ^{1}H NMR



23b. ^{13}C NMR

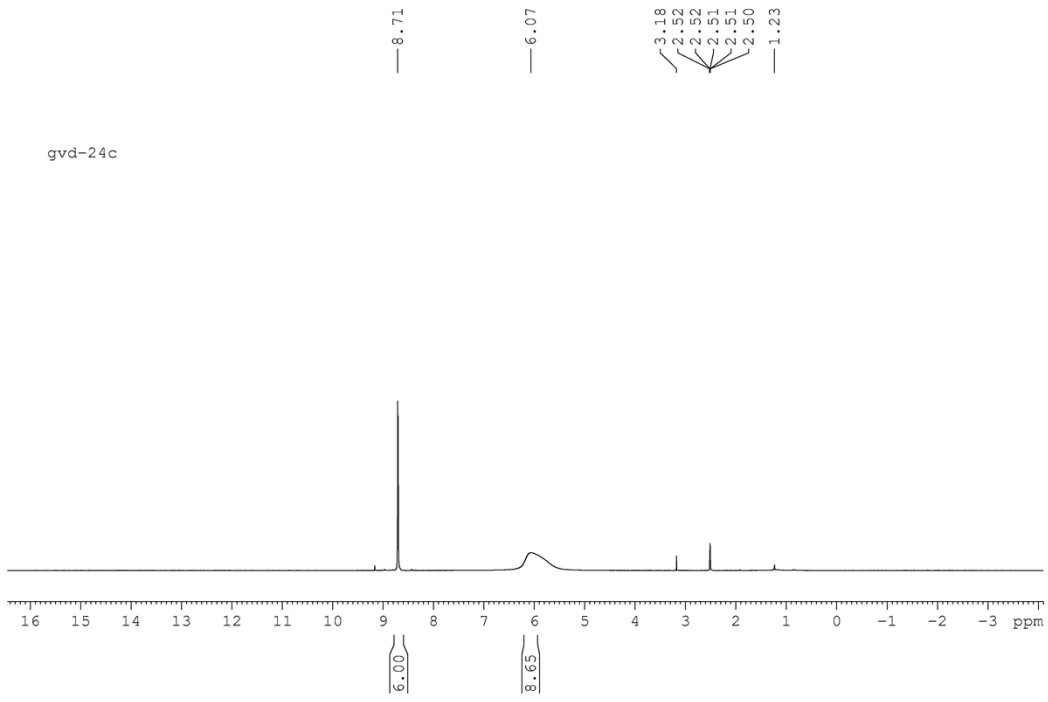


23c. TG-DTA

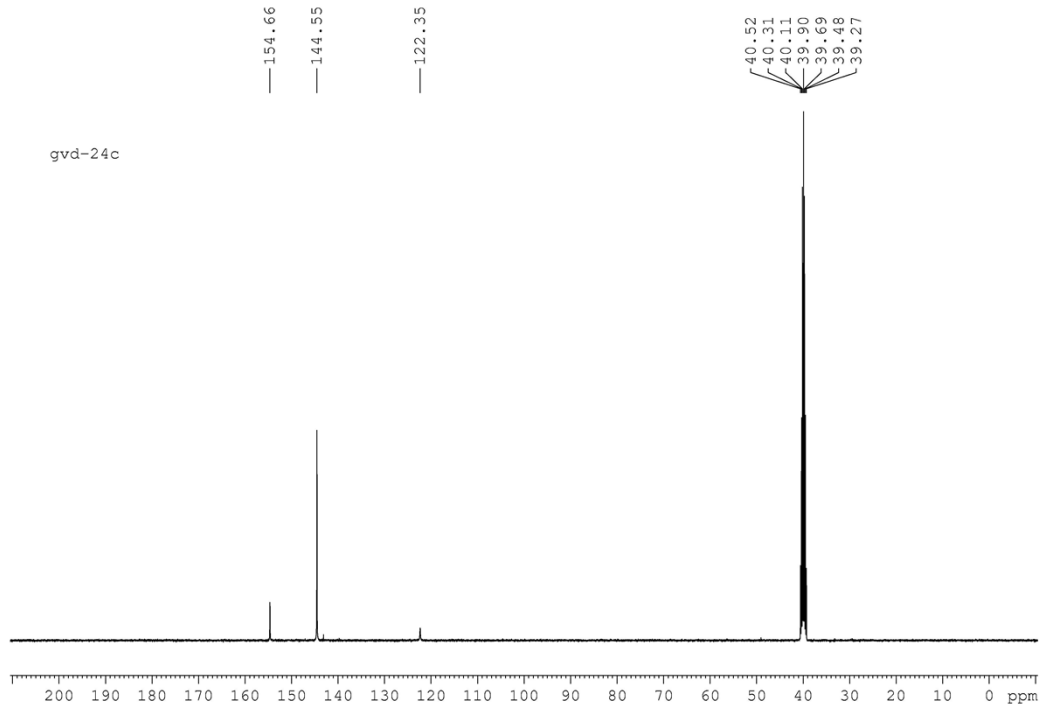


24. **Tris(4H-1,2,4-triazol-4-aminium) 2,4,6-trinitrobenzene-1,3,5-triolate (5a)**

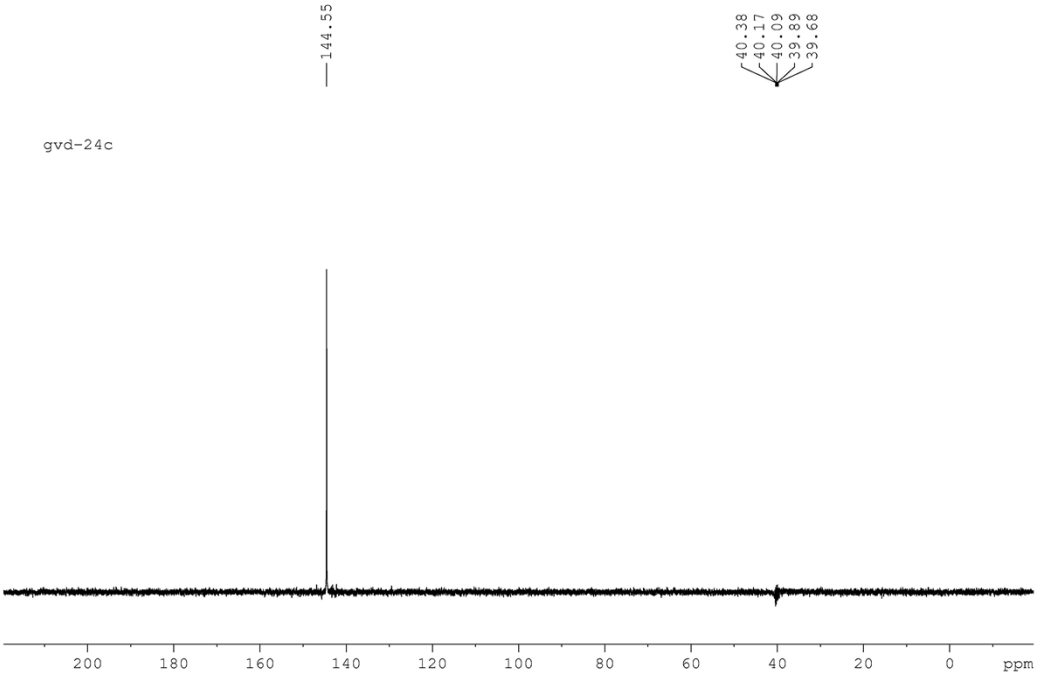
24a. ^{1}H NMR



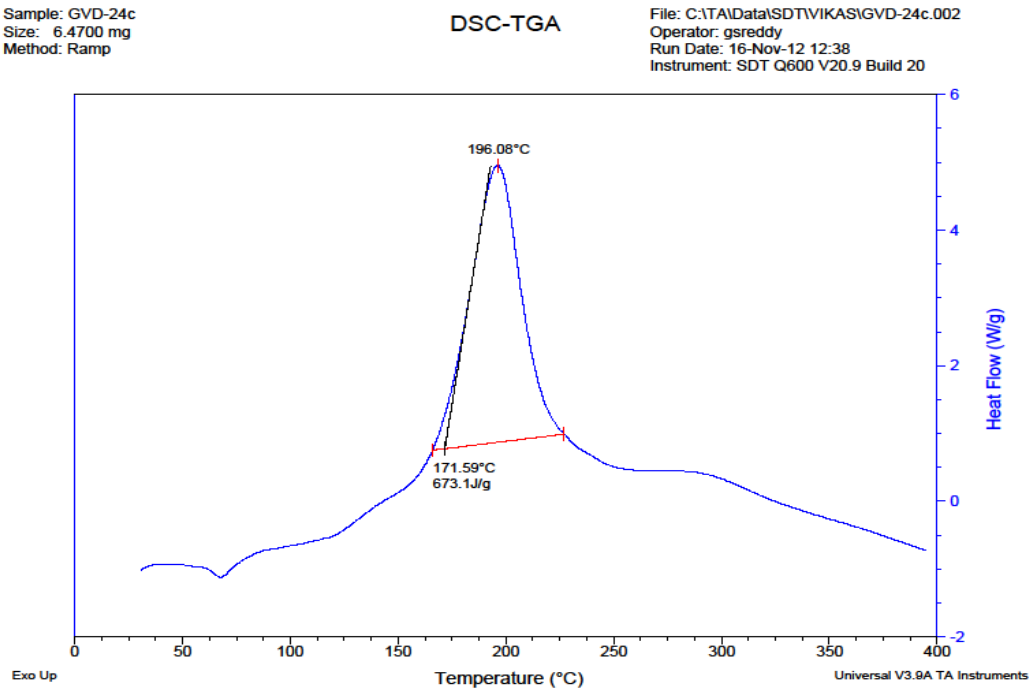
24b. ^{13}C NMR



24c. DEPT

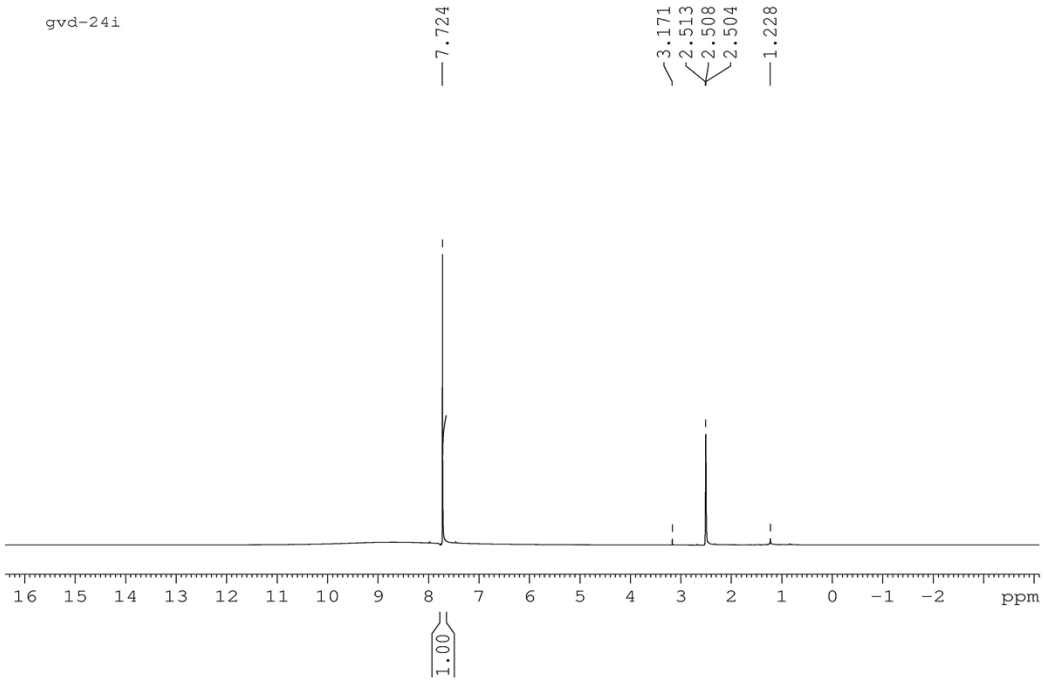


24d. TG-DTA

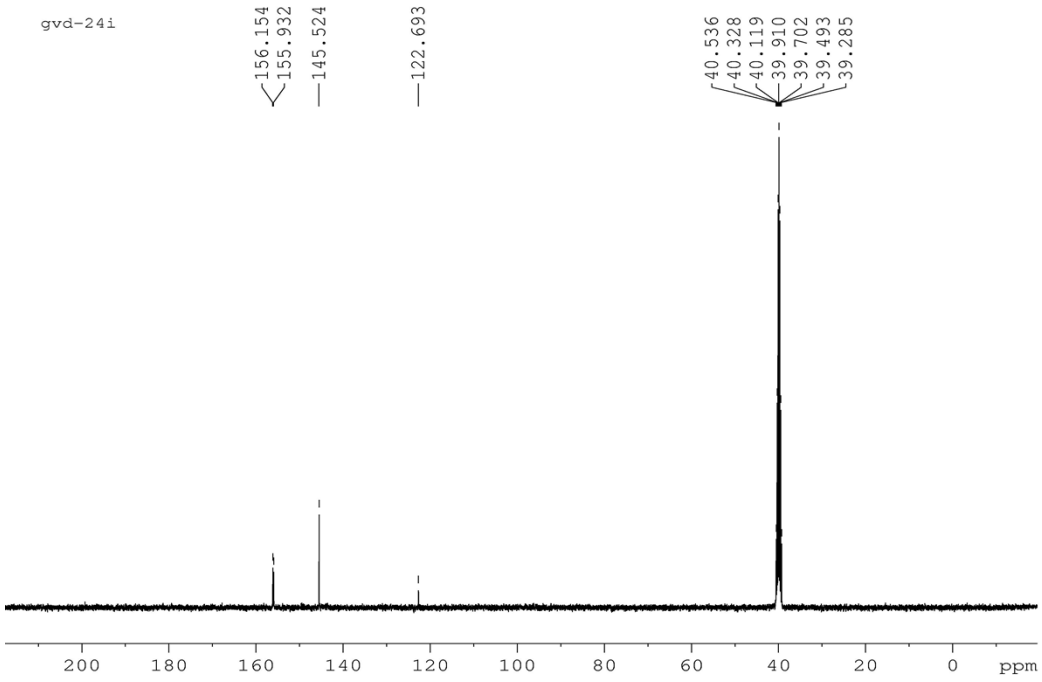


25. **Tris(3-amino-1H-1,2,4-triazol-4-ium) 2,4,6-trinitrobenzene-1,3,5-triolate (5b)**

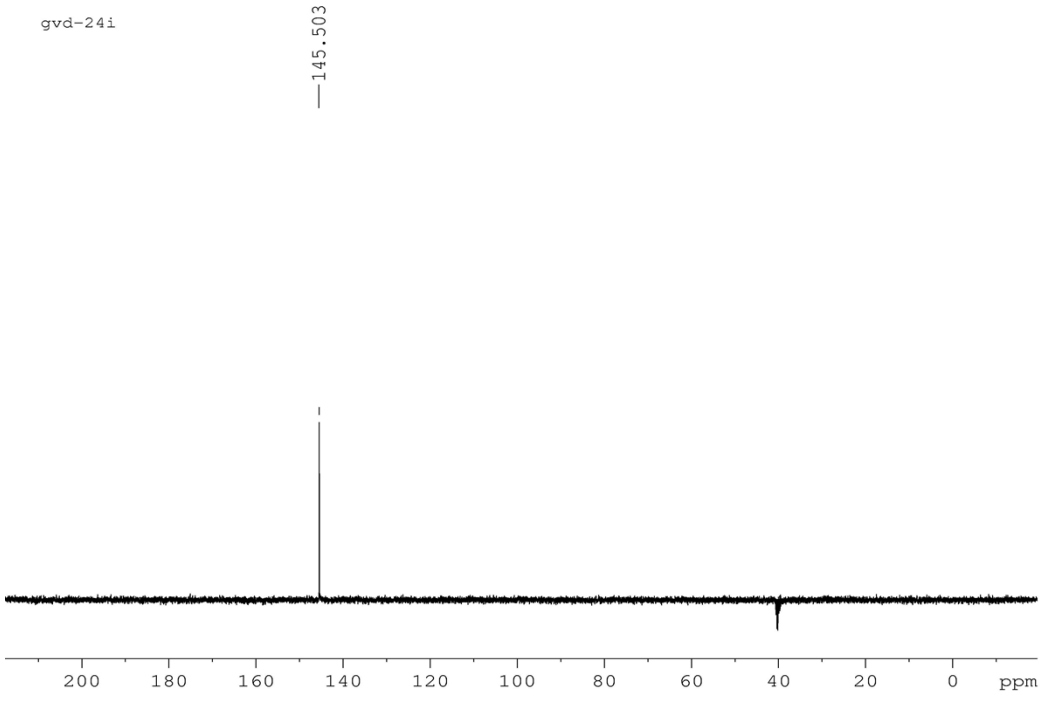
25a. ^{1}H NMR



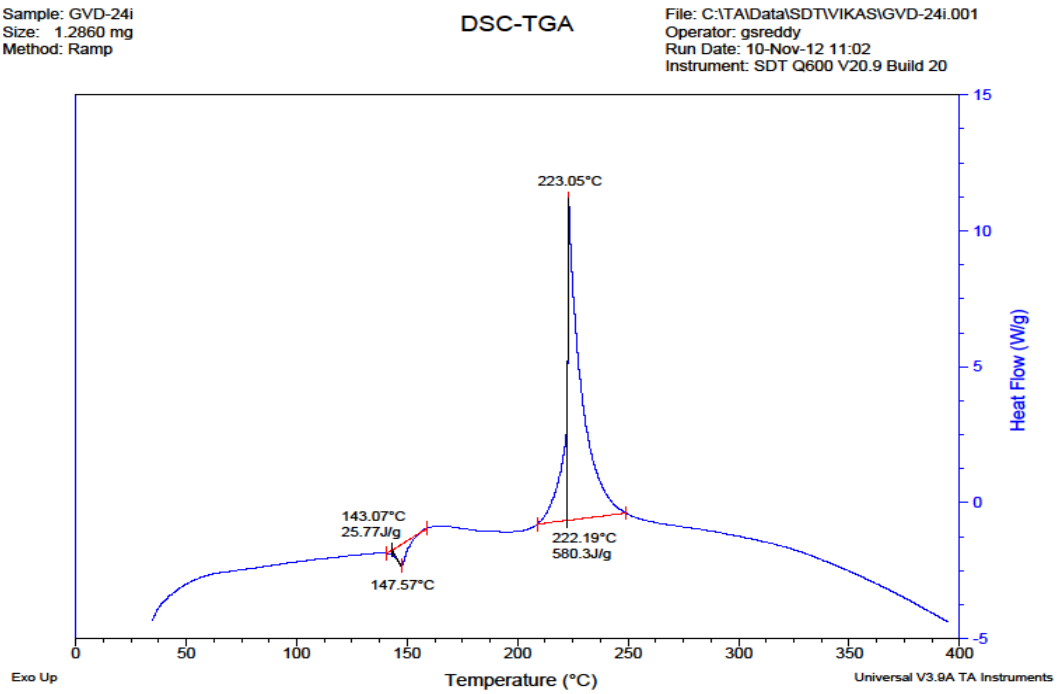
25b. ^{13}C NMR



25c. DEPT

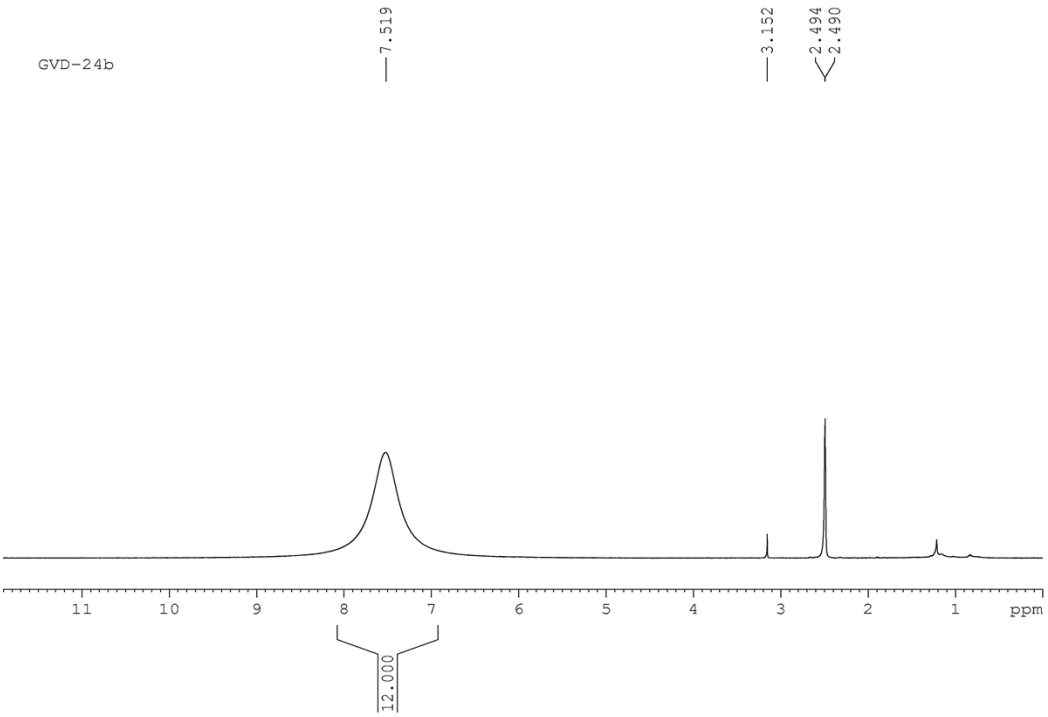


25d. TG-DTA

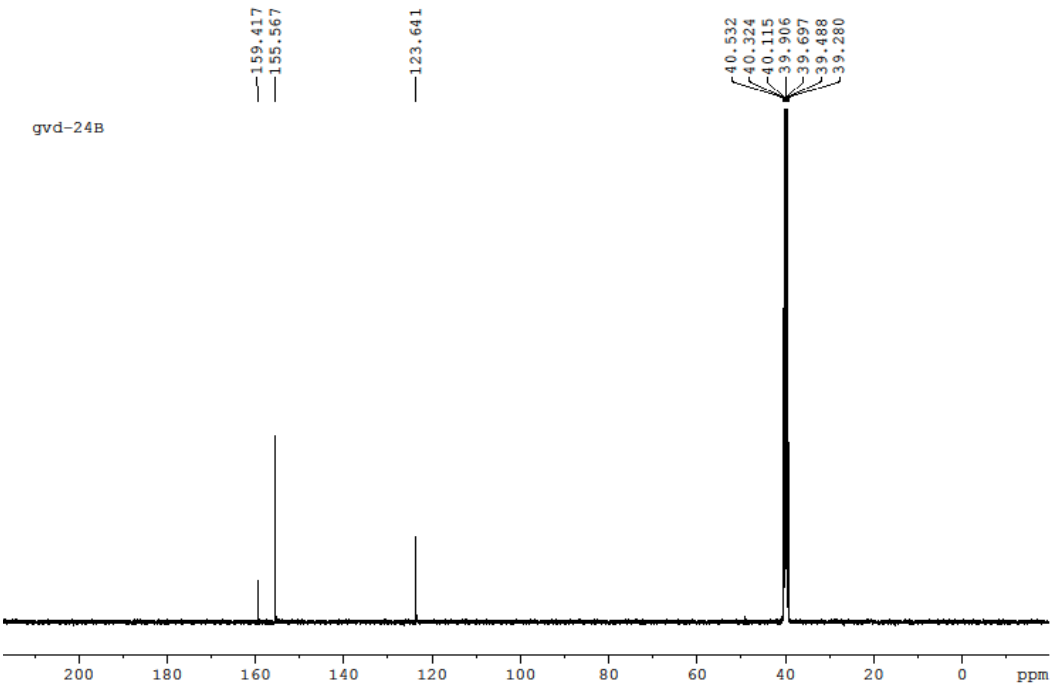


26. **Tris(3,5-diamino-1H-1,2,4-triazol-4-ium) 2,4,6-trinitrobenzene-1,3,5-triolate (5c)**

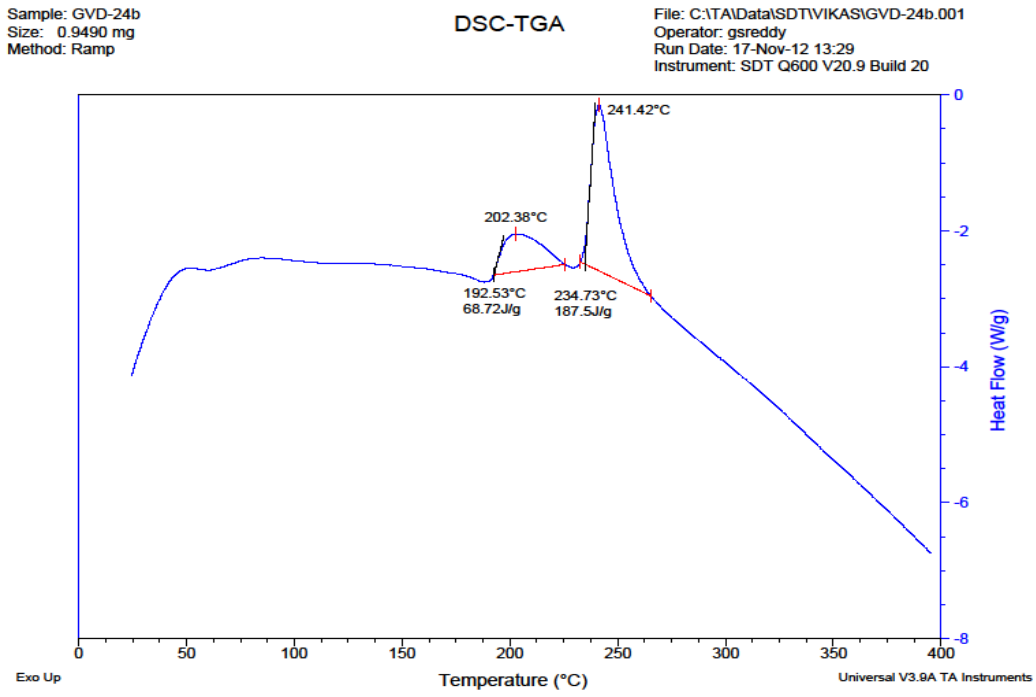
26a. ^{1}H NMR



26b. ^{13}C NMR

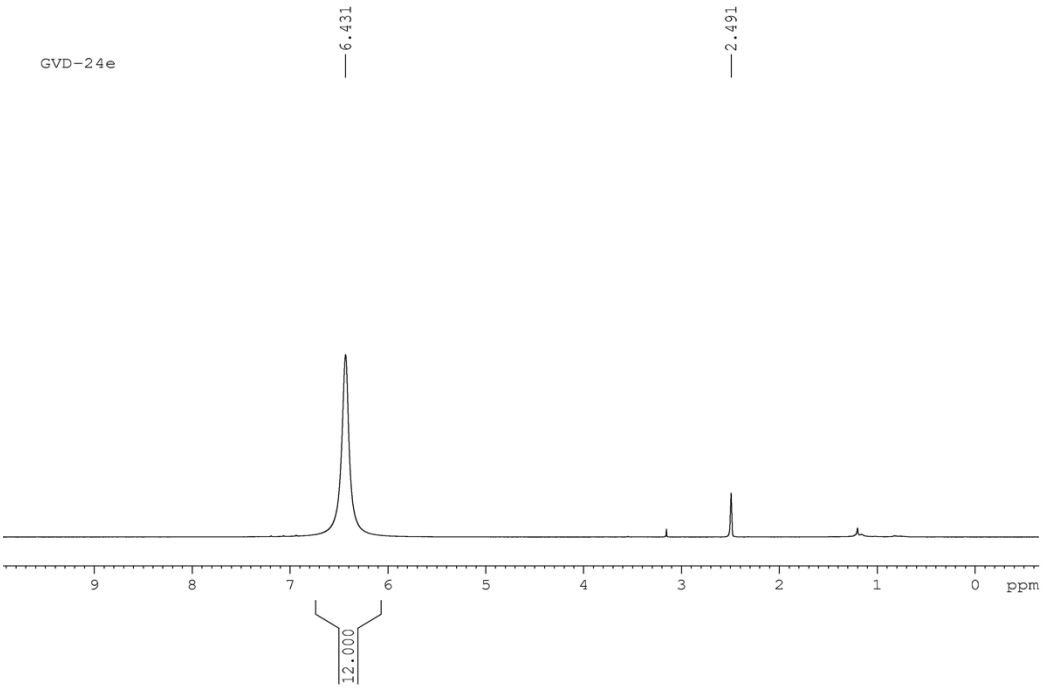


26c. TG-DTA

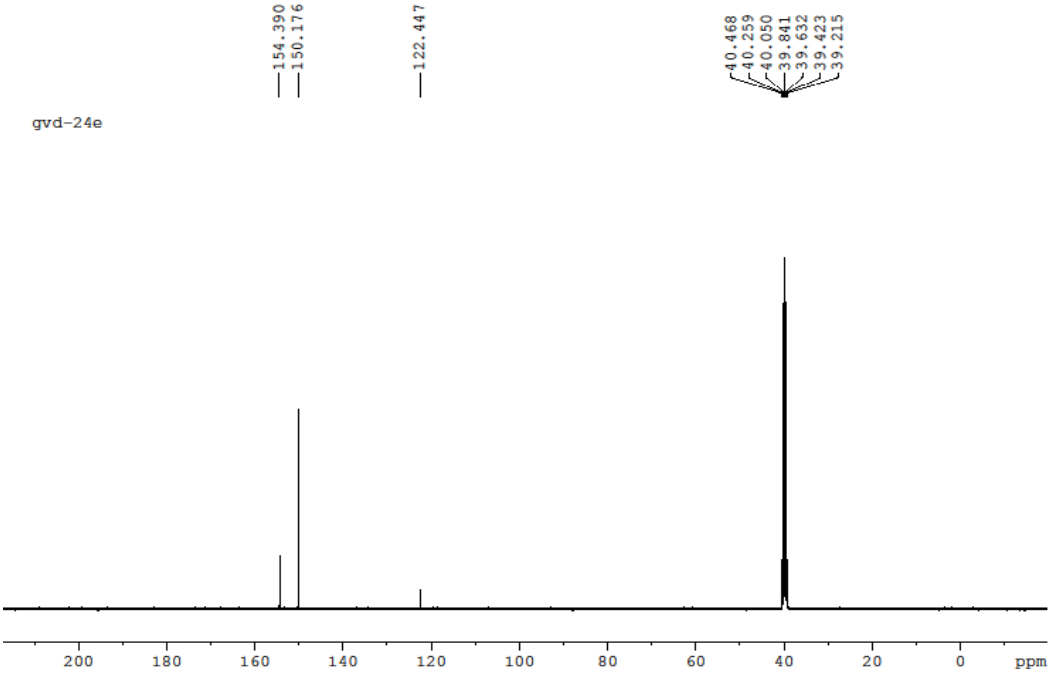


27. **Tris(3,4-diamino-1,2,5-oxadiazol-2-ium) 2,4,6-trinitrobenzene-1,3,5-triolate (5d)**

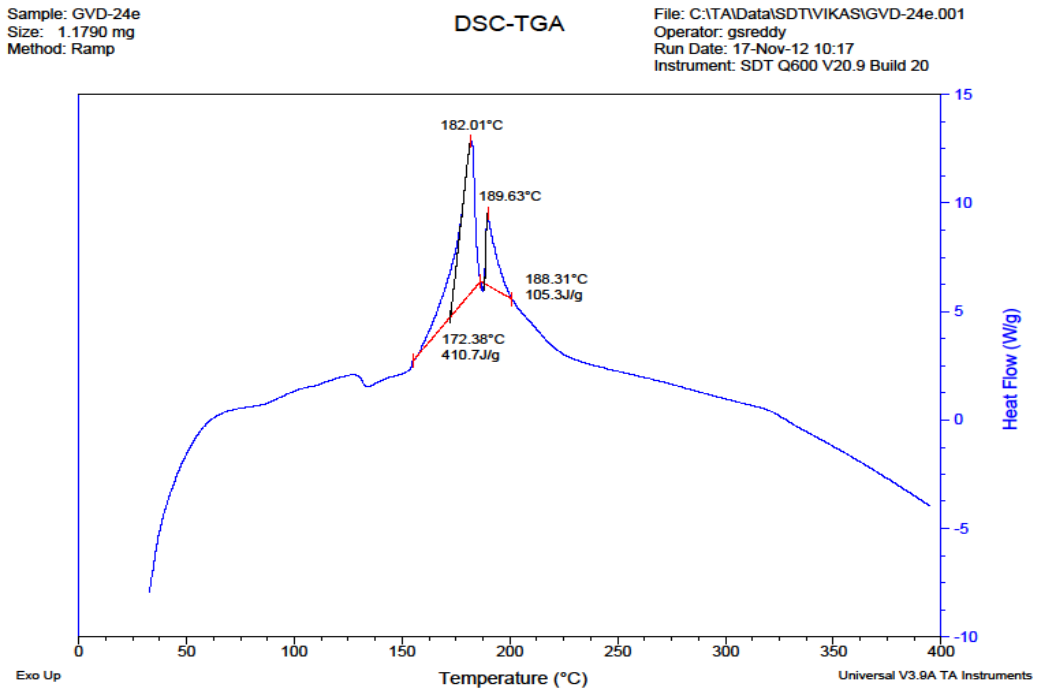
27a. ^{1}H NMR



27b. ^{13}C NMR

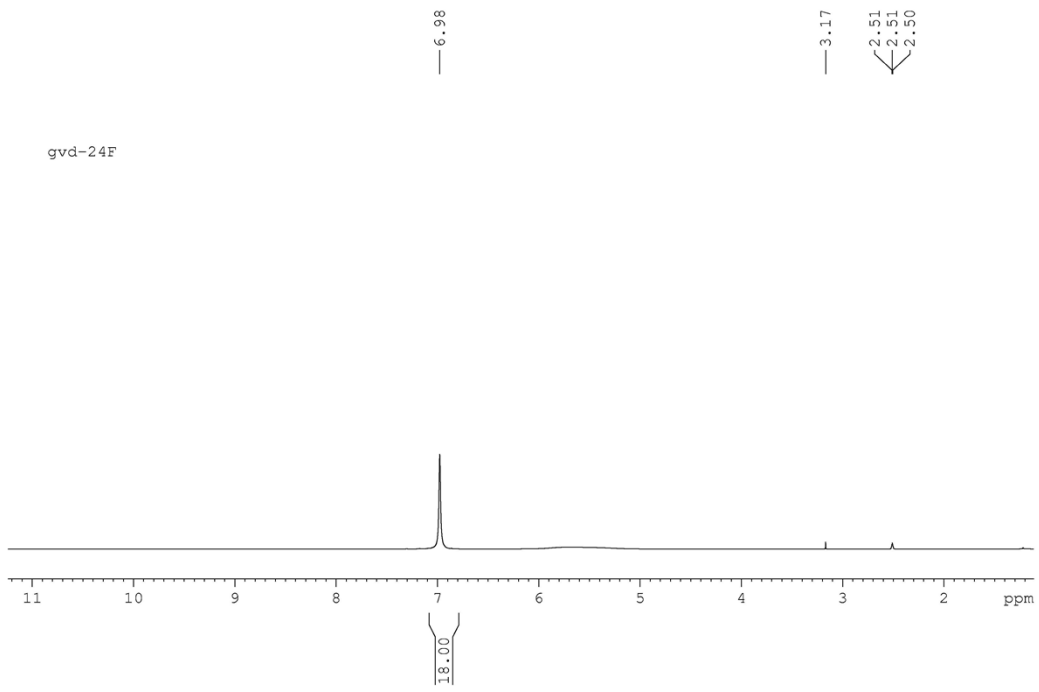


27c. TG-DTA

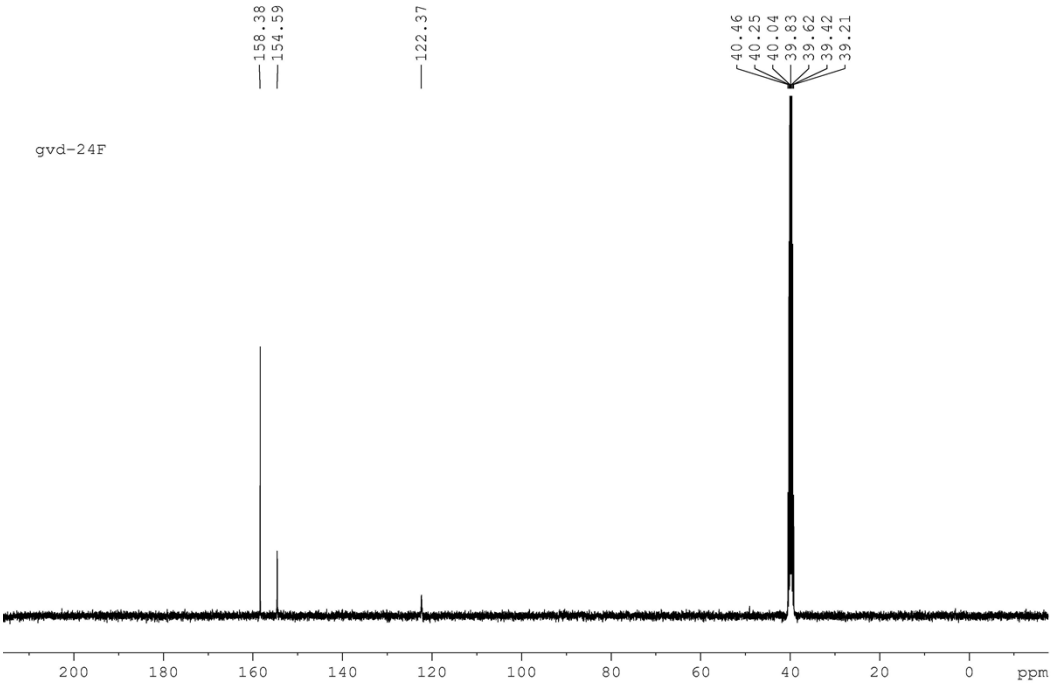


28. **Tris(diaminomethaniminium) 2,4,6-trinitrobenzene-1,3,5-triolate (5e)**

28a. ^{1}H NMR



28b. ^{13}C NMR



28c. TG-DTA