

## Supporting Information

### The 1,3,4,5-tetramino-1,2,4-triazolium Cation: An Energetic Moiety

Sebastian R. Yocca<sup>a,b,c</sup>, Joseph Yount<sup>b,c</sup>, Matthias Zeller<sup>d</sup>, Edward F. C. Byrd<sup>e</sup>, Davin G. Piercey<sup>b,c,f\*</sup>

<sup>a</sup> Department of Chemical Engineering, Purdue University, 480 Stadium Mall Drive, West Lafayette, IN, 47906, USA.

<sup>b</sup> Department of Materials Engineering, Purdue University, 205 Gates Road, West Lafayette, IN, 47906, USA.

<sup>c</sup> Purdue Energetics Research Center, Purdue University, 205 Gates Road, West Lafayette, IN, 47906, USA.

<sup>d</sup> Department of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN, 47906, USA.

<sup>e</sup> Detonation Sciences & Modeling Branch, CCDC U. S. Army Research Laboratory, Aberdeen Proving Ground, MD, 21005, USA.

<sup>f</sup> Department of Mechanical Engineering, Purdue University, 585 Purdue Mall, West Lafayette, IN, 47906, USA.

\*Corresponding Author: [dpiercey@purdue.edu](mailto:dpiercey@purdue.edu)

<b>Table of Contents</b>	<b>Page</b>
<b>1. IR spectra</b>	<b>S2</b>
<b>2. <sup>1</sup>H NMR spectra</b>	<b>S4</b>
<b>3. <sup>13</sup>C NMR spectra</b>	<b>S8</b>
<b>4. <sup>15</sup>N NMR spectrum</b>	<b>S11</b>
<b>5. TGA-DSC spectra</b>	<b>S12</b>

# 1. IR spectra

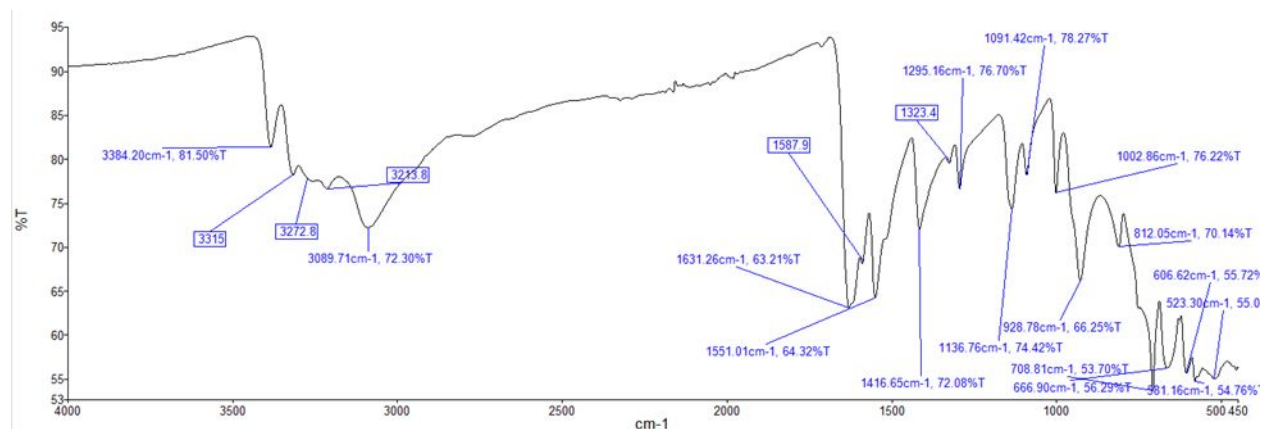
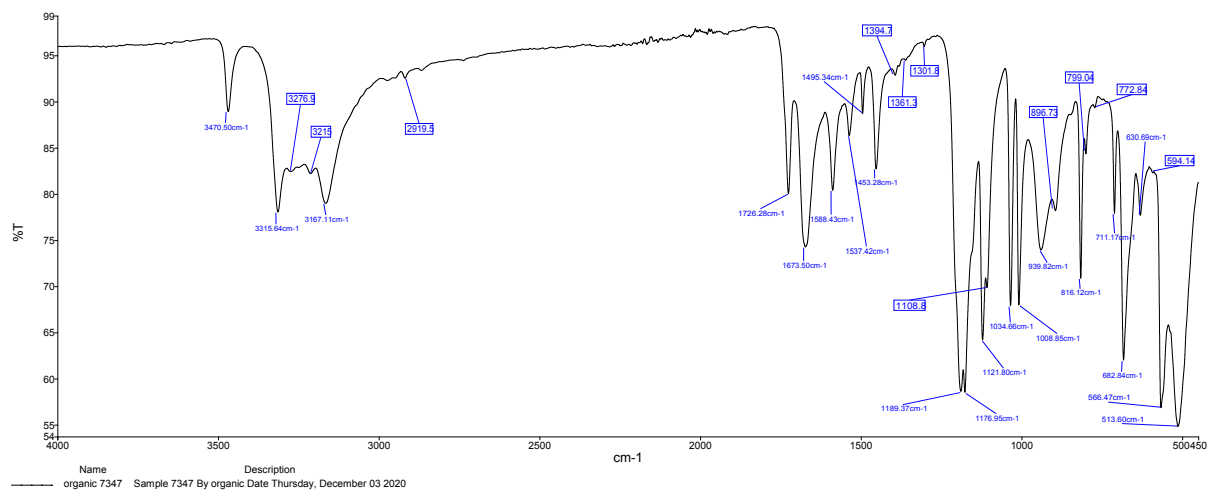
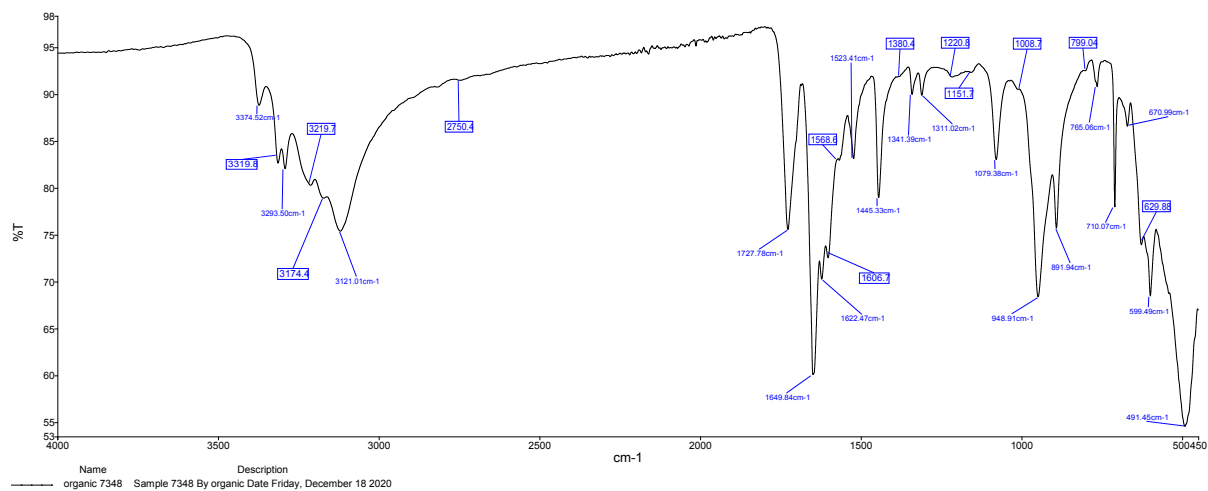


Figure S1. Infrared spectrum of 3,4,5-triamino-1,2,4-triazole.



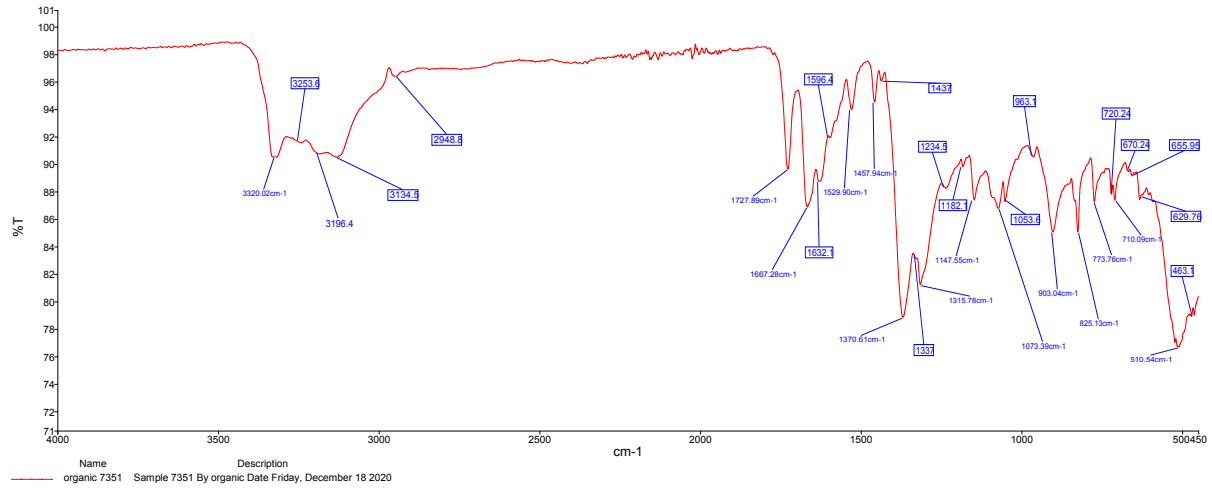
Name: organic 7347  
Description: Sample 7347 By organic  
Date: Thursday, December 03 2020

Figure S2. Infrared spectrum of salt 1.

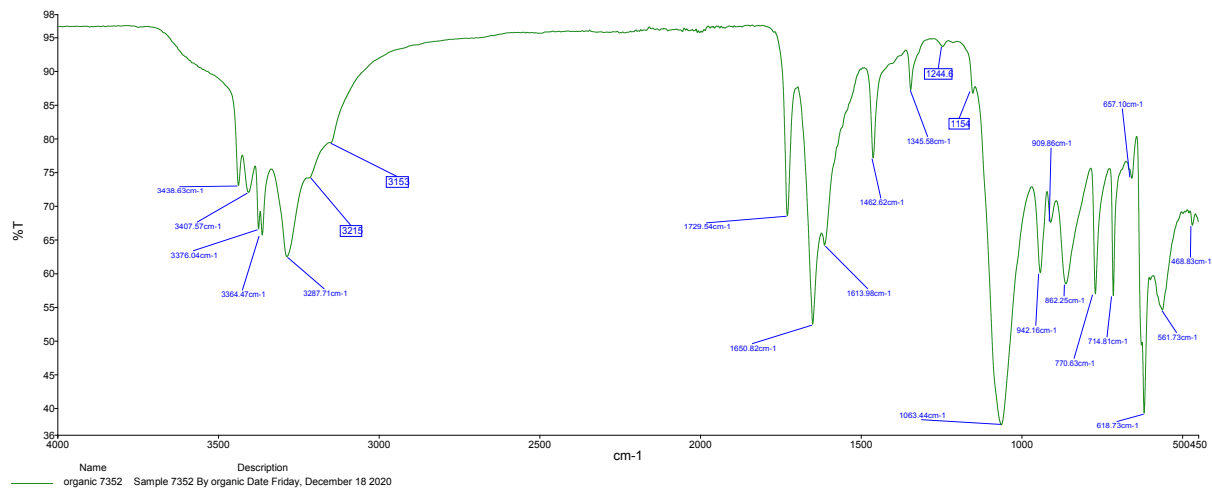


Name: organic 7348  
Description: Sample 7348 By organic  
Date: Friday, December 18 2020

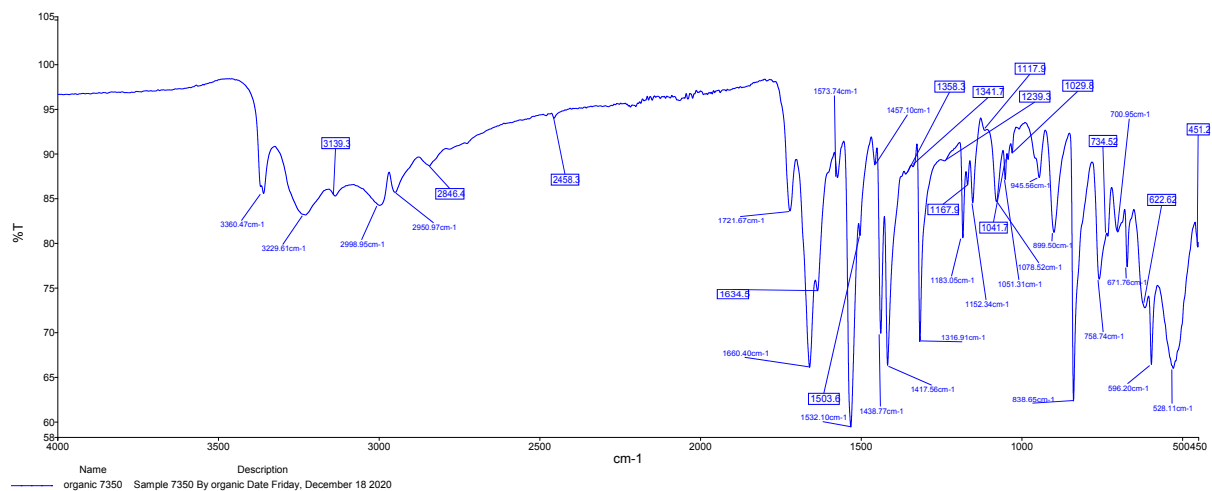
Figure S3. Infrared spectrum of salt 2.



**Figure S4. Infrared spectrum of salt 3.**



**Figure S5. Infrared spectrum of salt 4.**



**Figure S6. Infrared spectrum of salt 5.**

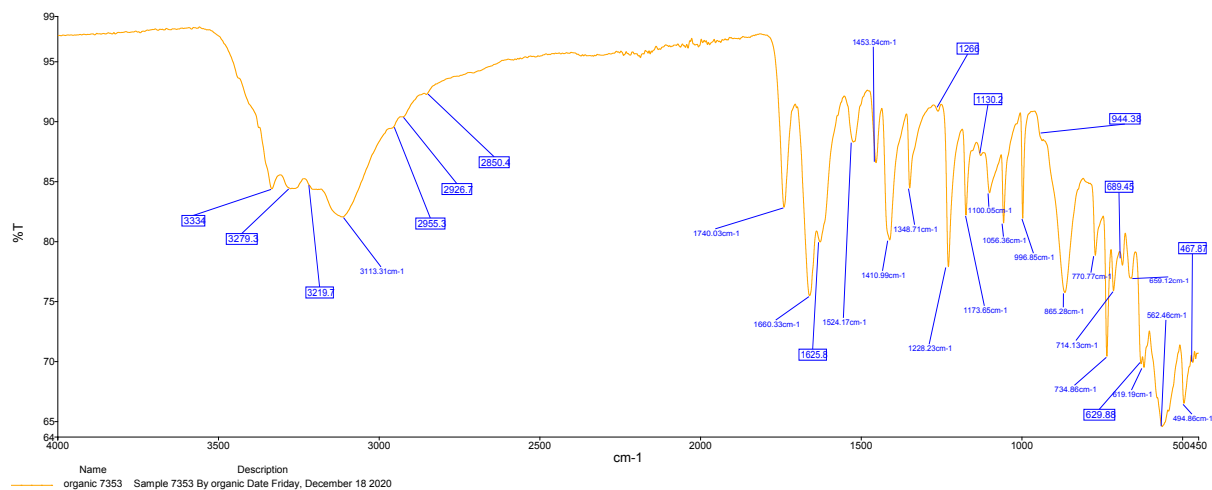


Figure S7. Infrared spectrum of salt 6.

## 2. <sup>1</sup>H NMR spectra

Resonances appearing around 2.5 ppm and 3.3 ppm correspond to the solvent DMSO and trace amounts of water respectively.

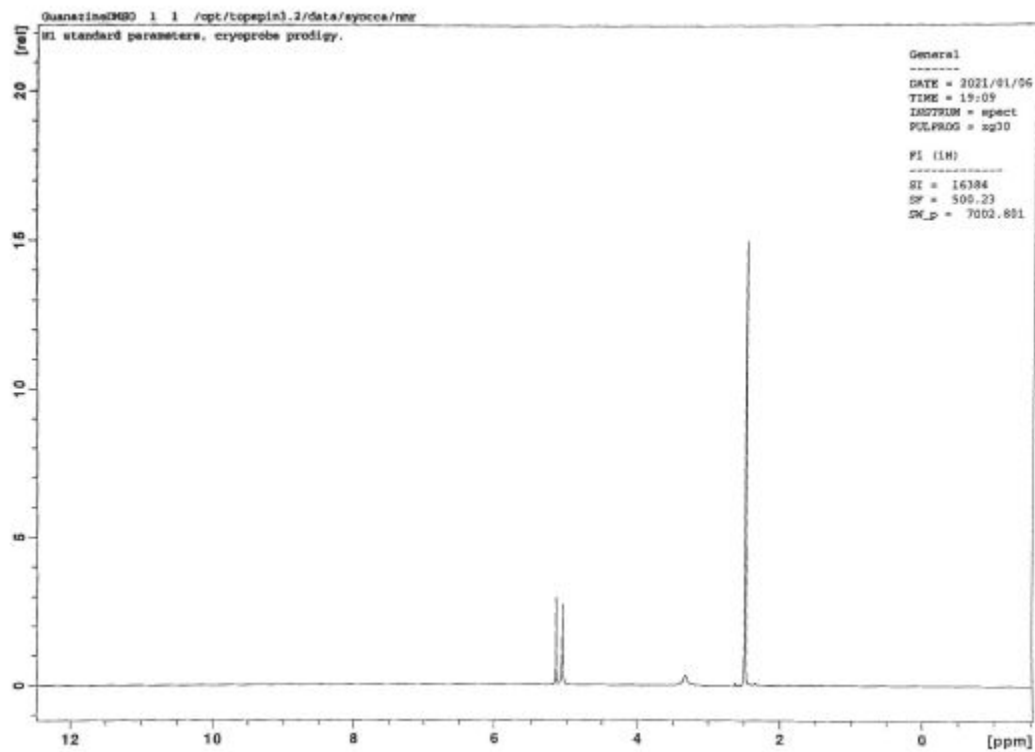


Figure S8. <sup>1</sup>H NMR spectrum of 3,4,5-triamino-1,2,4-triazole.

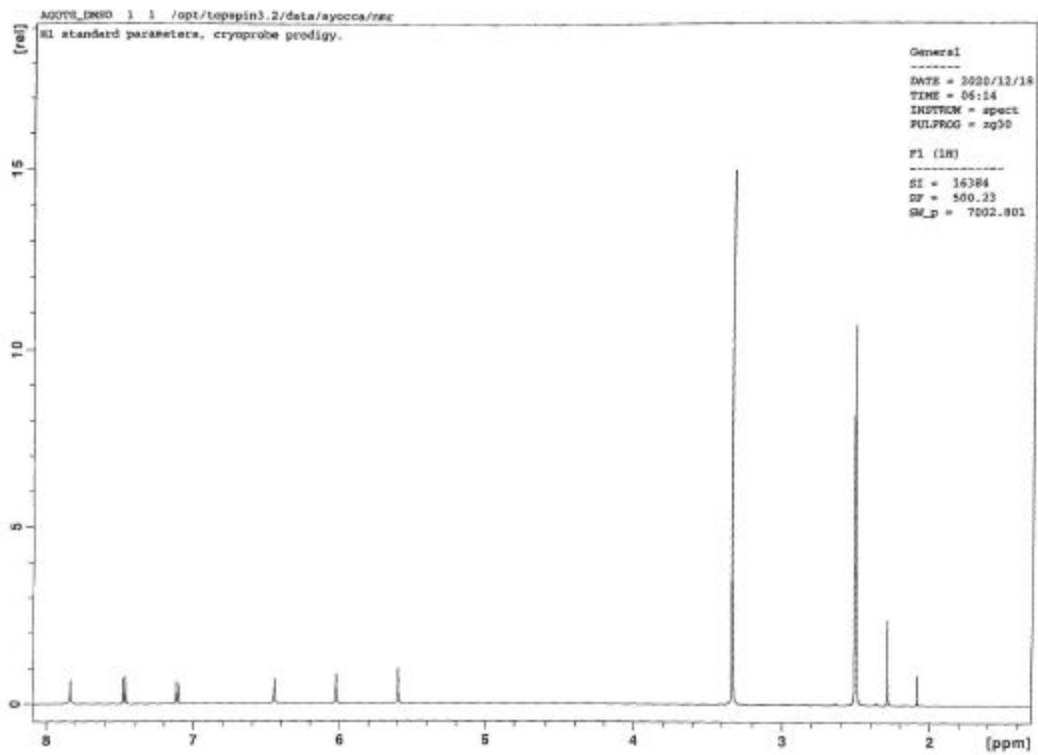


Figure S9.  $^1\text{H}$  NMR spectrum of salt 1.

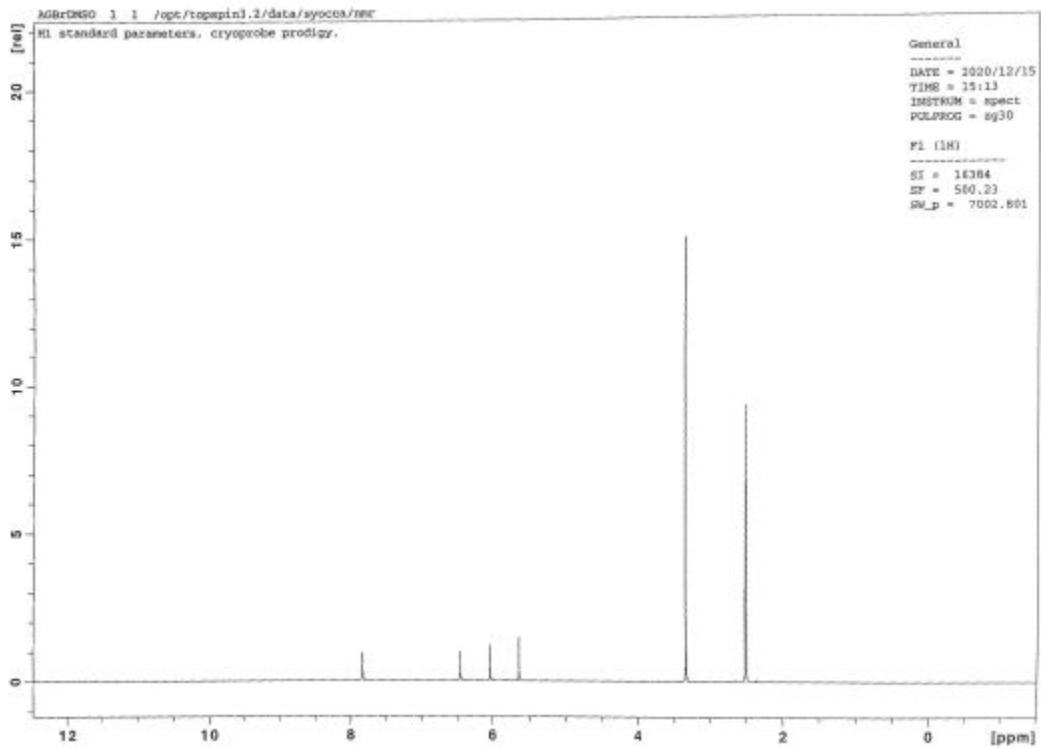


Figure S10.  $^1\text{H}$  NMR spectrum of salt 2.

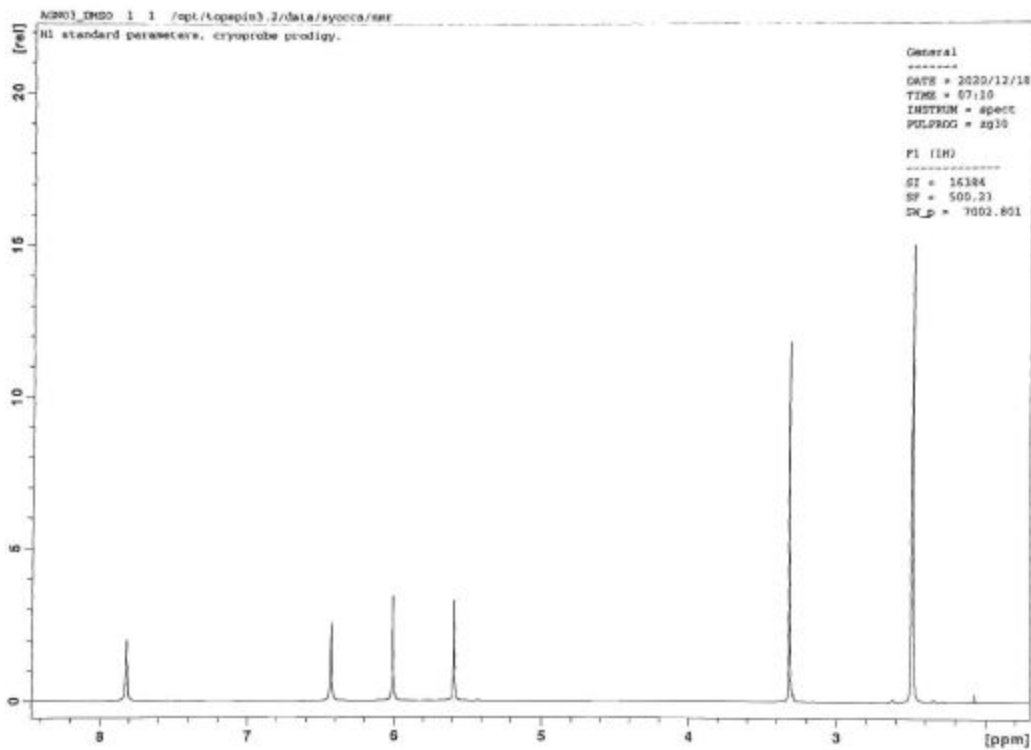


Figure S11.  $^1\text{H}$  NMR spectrum of salt 3.

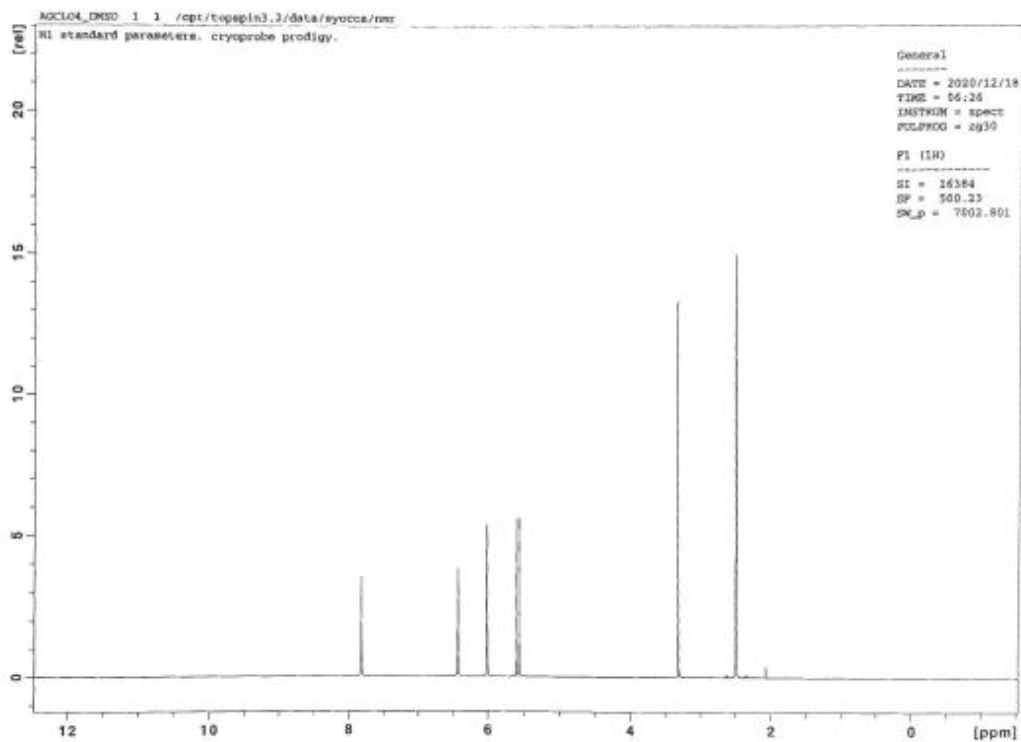


Figure S12.  $^1\text{H}$  NMR spectrum of salt 4.

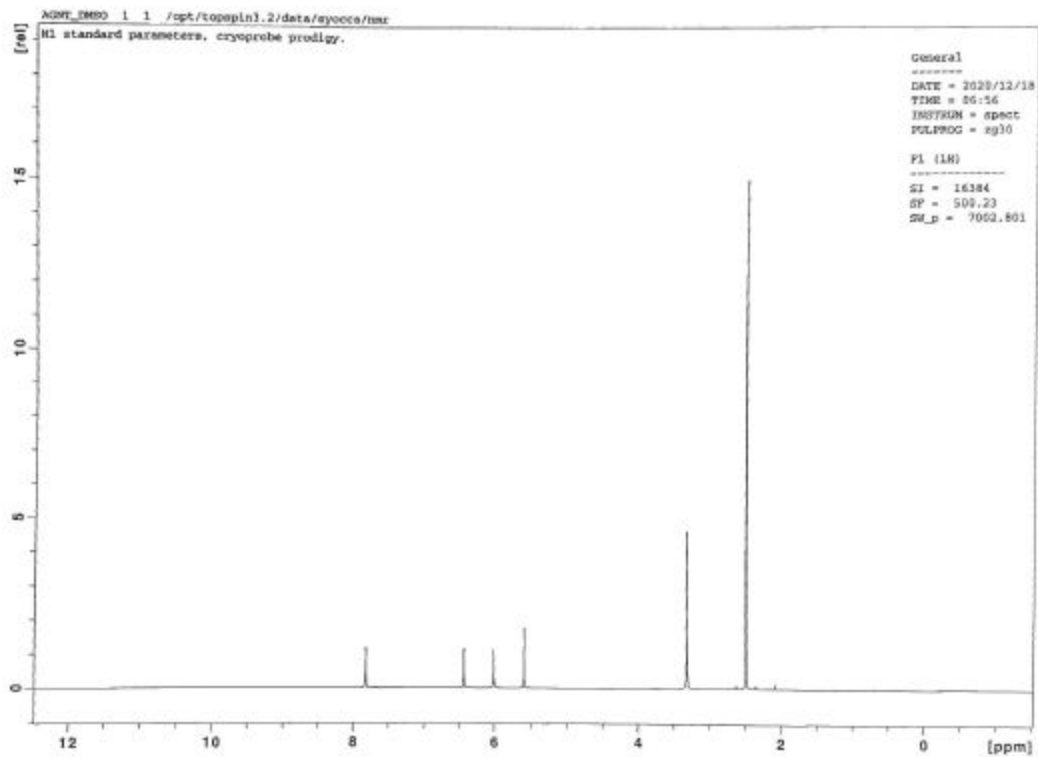


Figure S13.  $^1\text{H}$  NMR spectrum of salt 5.

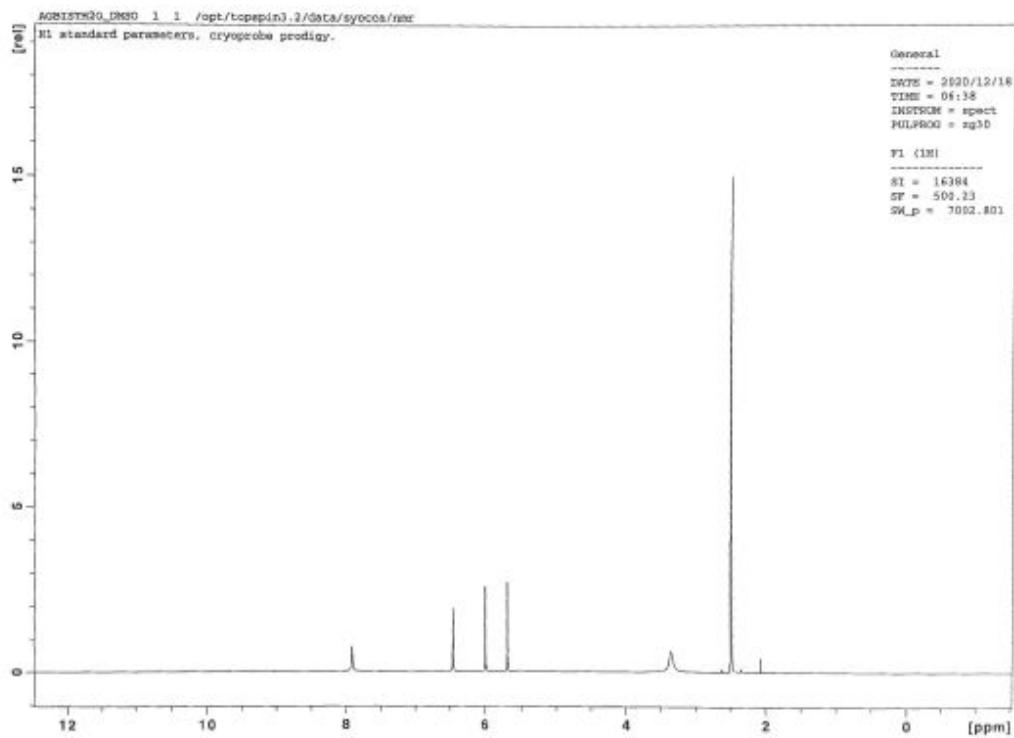


Figure S14.  $^1\text{H}$  NMR spectrum of salt 6.

### 3. $^{13}\text{C}$ NMR spectra

The resonance near 40.0 ppm corresponds to the solvent, DMSO.

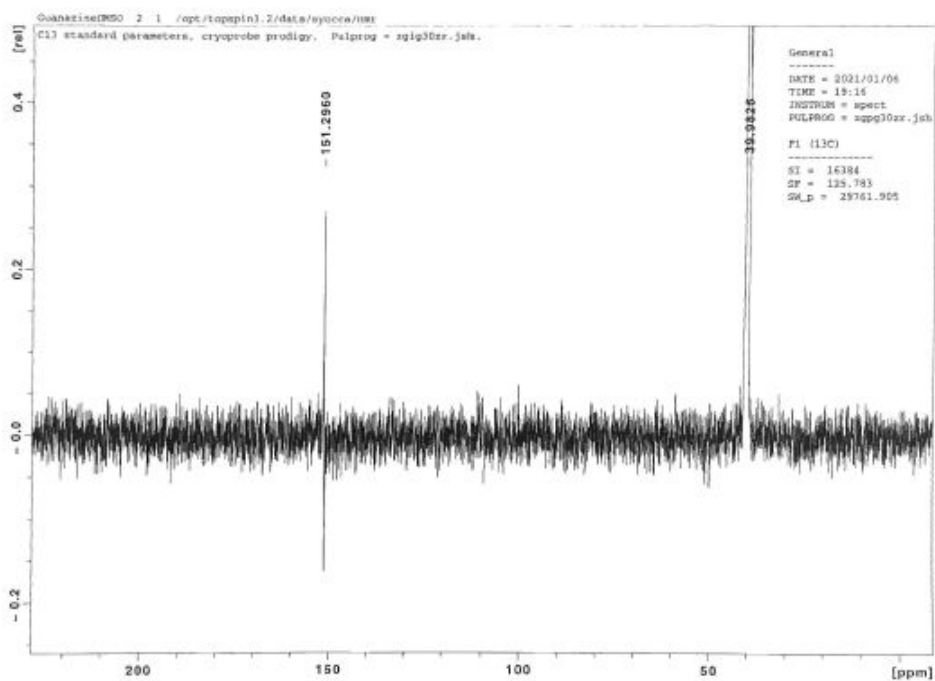


Figure S15.  $^{13}\text{C}$  NMR spectrum of 3,4,5-triamino-1,2,4-triazole.

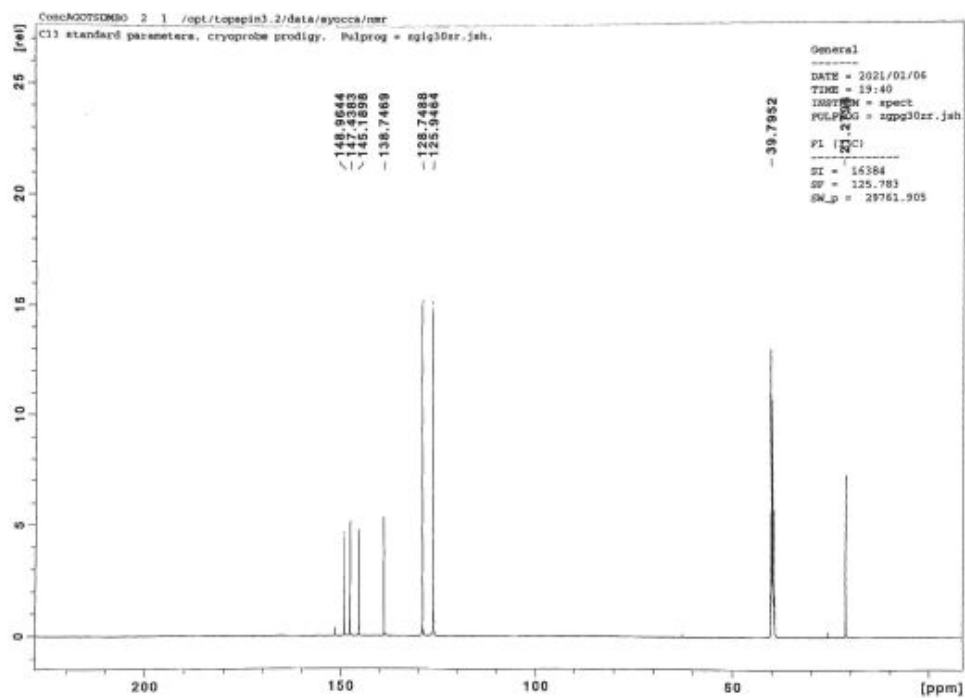


Figure S16.  $^{13}\text{C}$  NMR spectrum of salt 1.



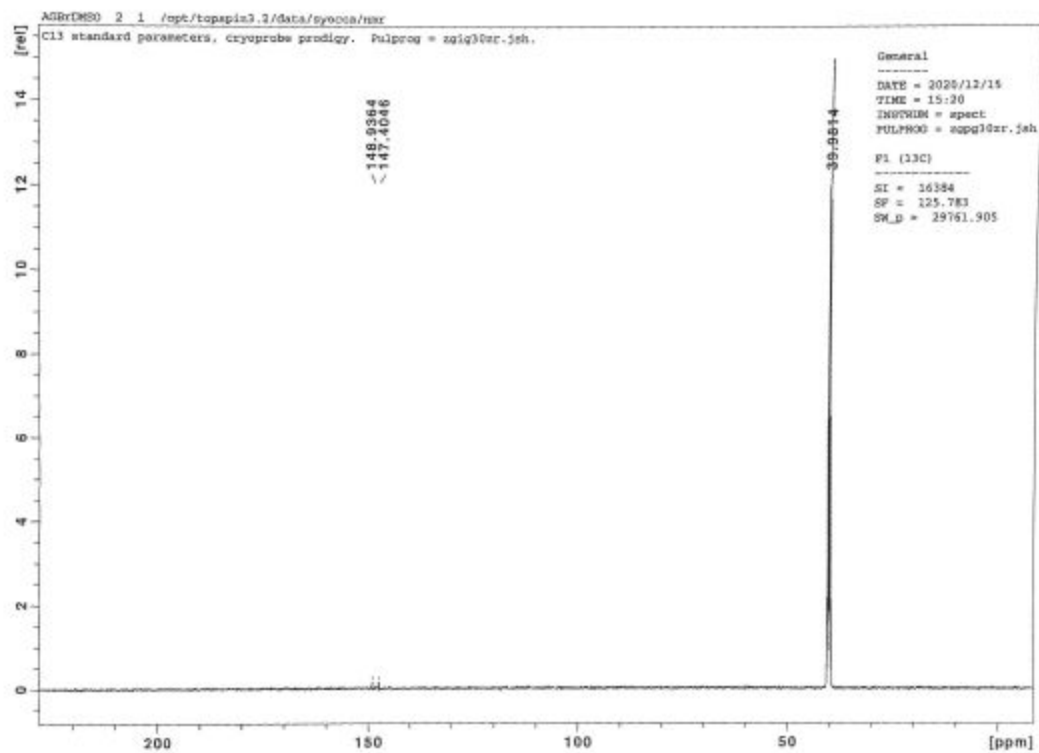


Figure S17.  $^{13}\text{C}$  NMR spectrum of salt 2.

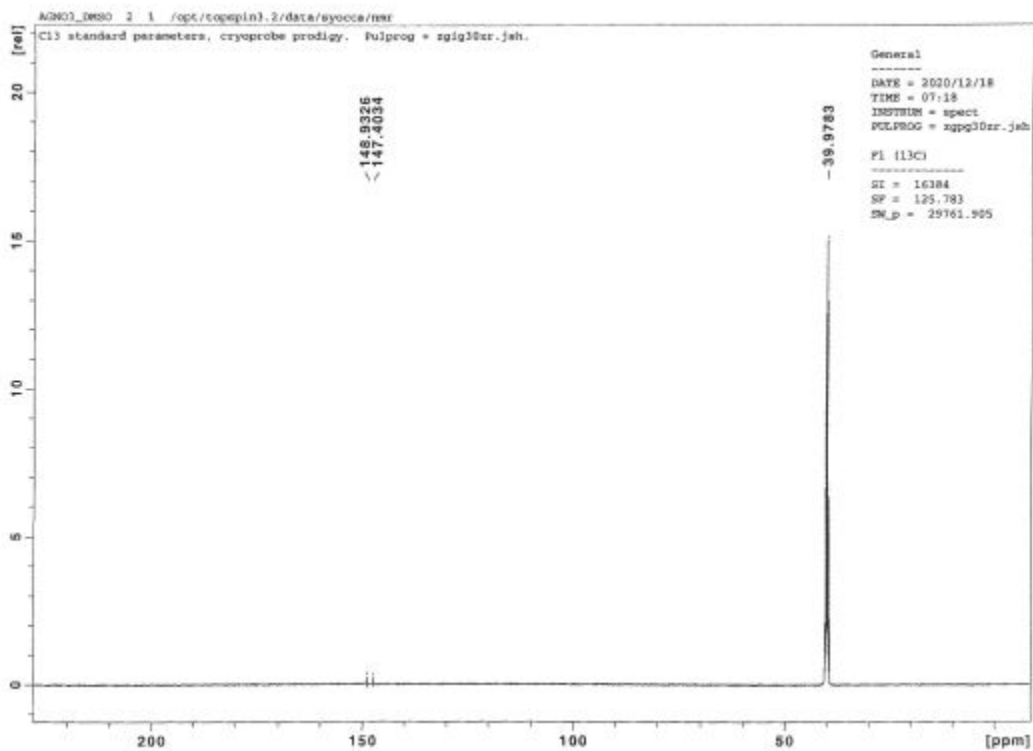


Figure S18.  $^{13}\text{C}$  NMR spectrum of salt 3.

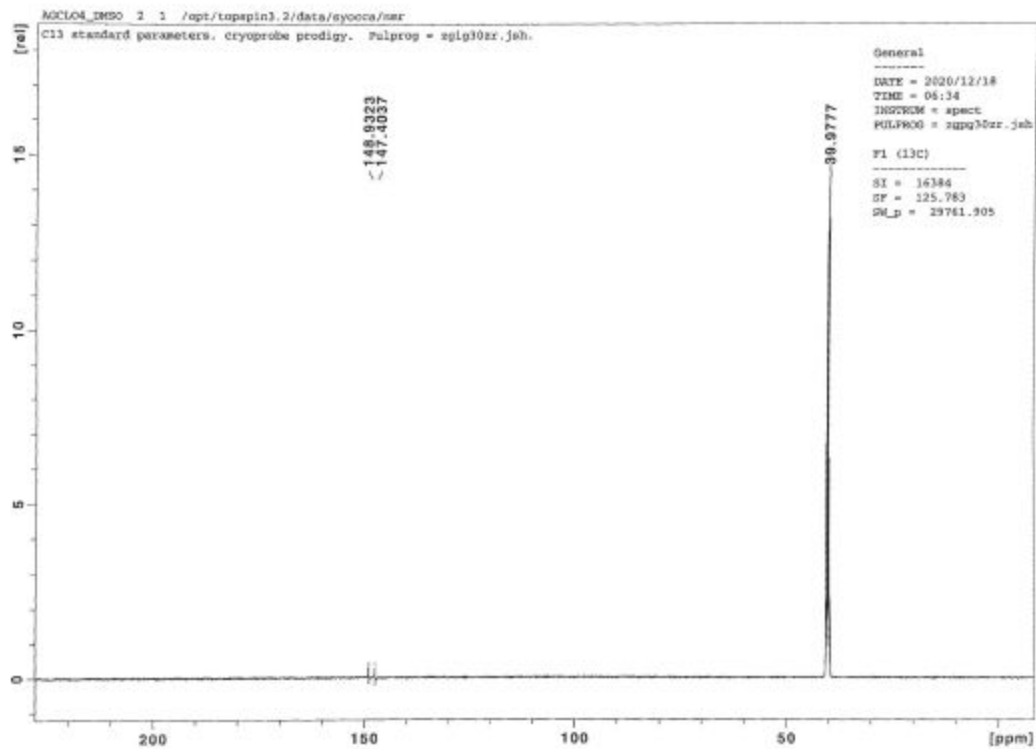


Figure S19.  $^{13}\text{C}$  NMR spectrum of salt 4.

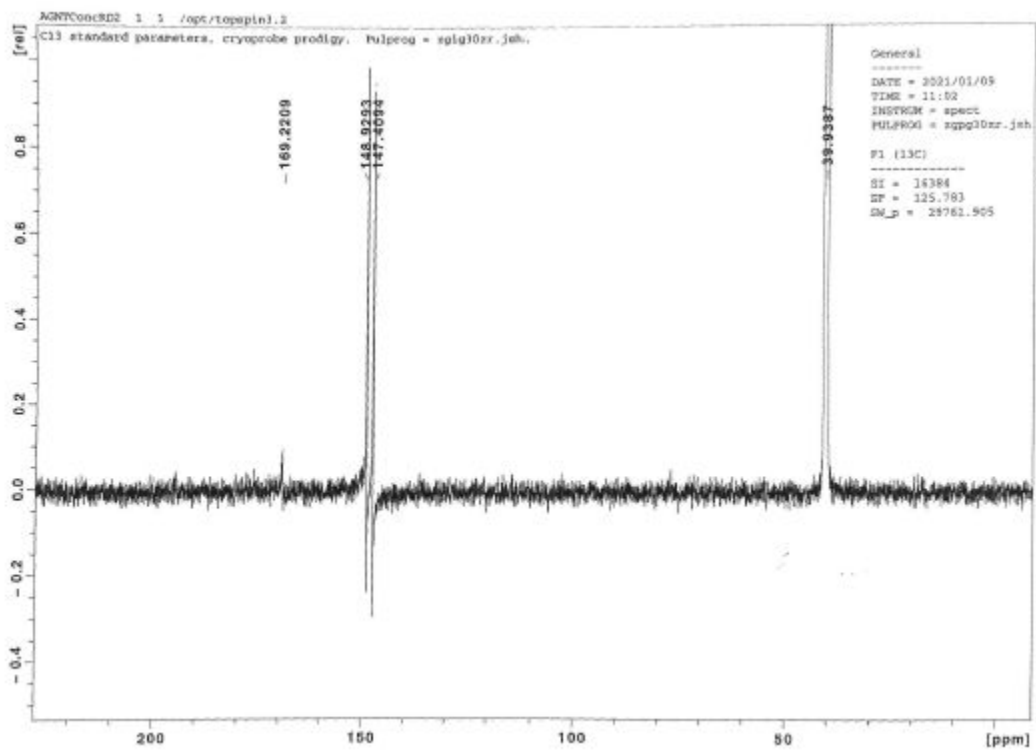


Figure S20.  $^{13}\text{C}$  NMR spectrum of salt 5.

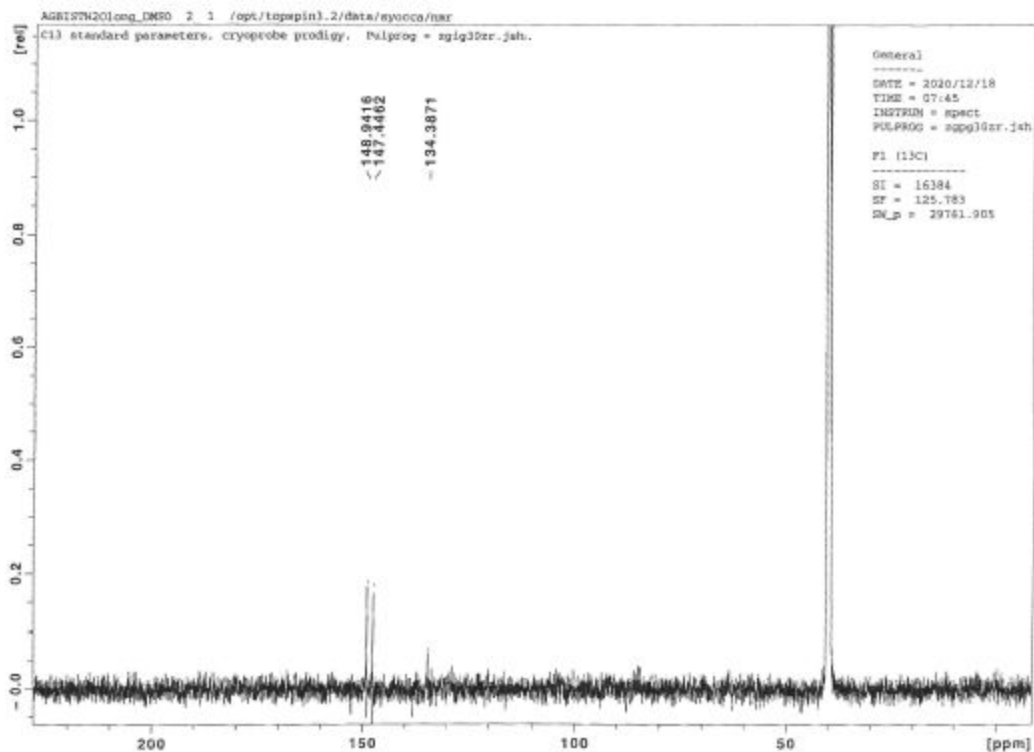


Figure S21.  $^{13}\text{C}$  NMR spectrum of salt 6.

#### 4. $^{15}\text{N}$ NMR spectrum

Acquisition parameters for this spectrum were as follows: zgig30 pulse sequence, sweep width 500 ppm, D1 3 sec, TD 64000, 4096 scans, 1.3 sec acquisition time, 144 receiver gain, inverse-gated decoupling.

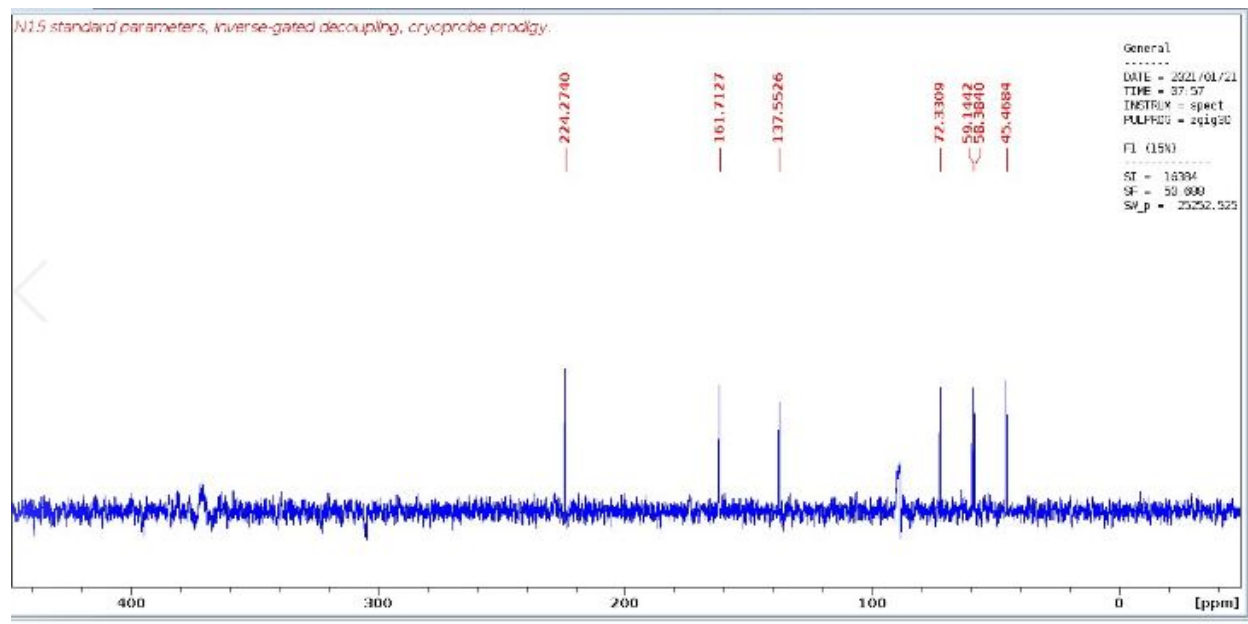


Figure S22.  $^{15}\text{N}$  NMR spectrum of salt 1.

## 5. TGA-DSC spectra

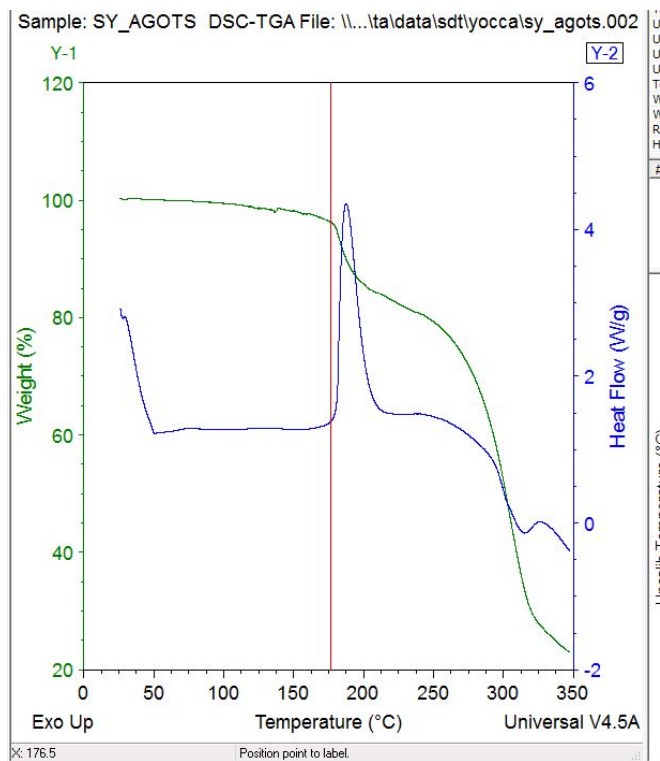
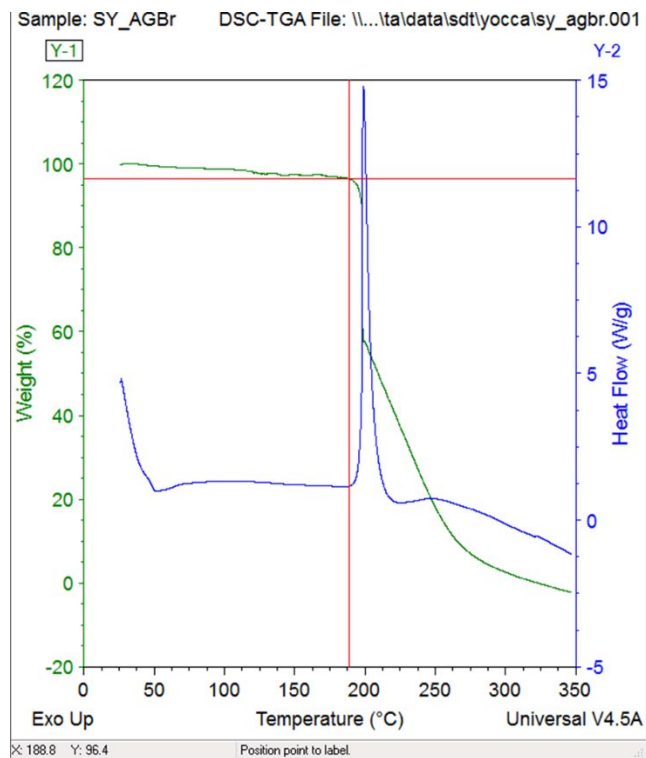
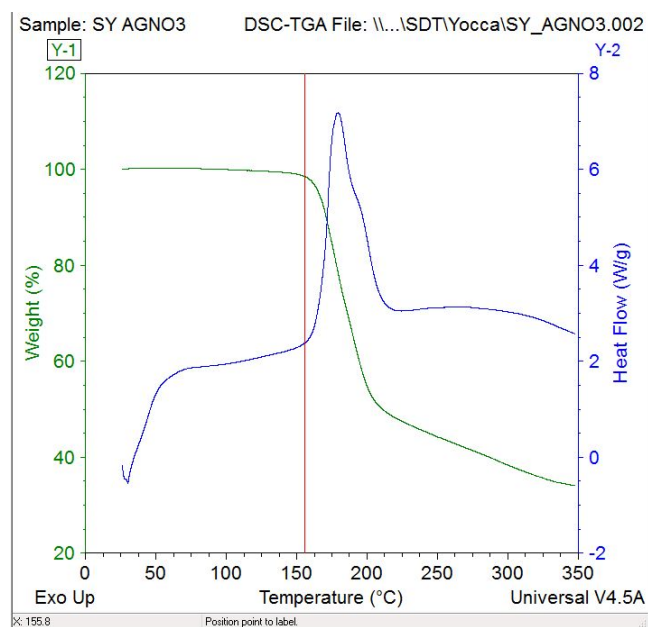


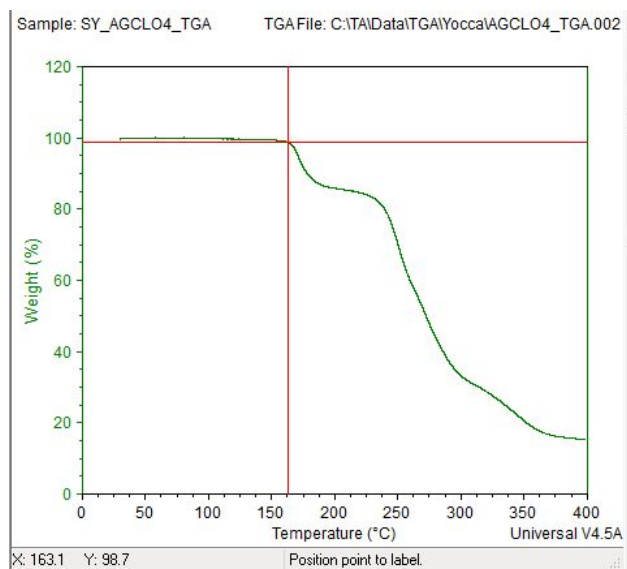
Figure S23. Thermal decomposition (DSC) spectrum of salt 1.



**Figure S24.** Thermal decomposition (DSC) spectrum of salt 2.



**Figure S25.** Thermal decomposition (DSC) spectrum of salt 3.



**Figure S26.** Thermal decomposition (TGA) spectrum of salt 4.

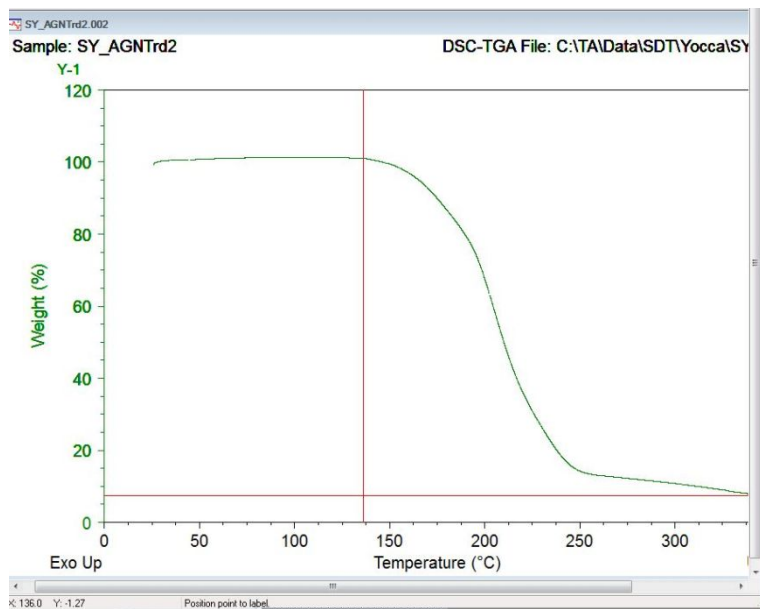


Figure S27. Thermal decomposition (TGA) spectrum of salt 5.

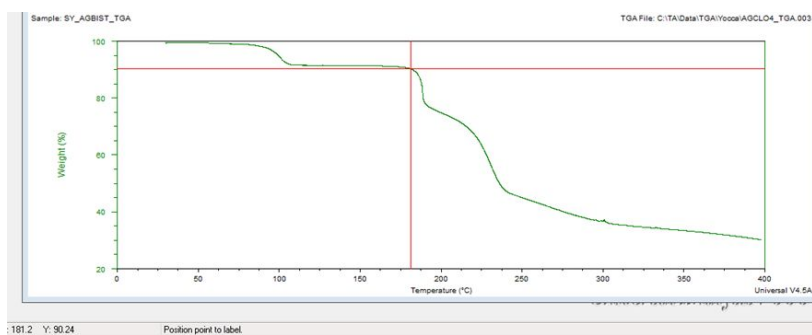


Figure S28. Thermal decomposition (TGA) spectrum of salt 6.