

Supporting Information

## Process Development, Friction Insensitivity Improvement and Compatibility Studies of Tetranitroacetimidic Acid

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### 1. Synthesis of TNAA

Nitration of 1,1-diamino-2,2-dinitroethene (FOX-7) was carried out at ambient condition using excess fuming nitric acid in various proportions ranging from 14 to 50 per mole of FOX-7. TNAA was obtained on evacuating excess nitric acid and crystallization from dichloromethane as white solid.

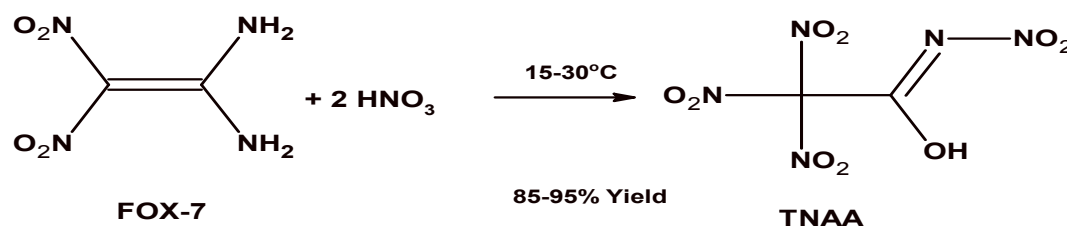
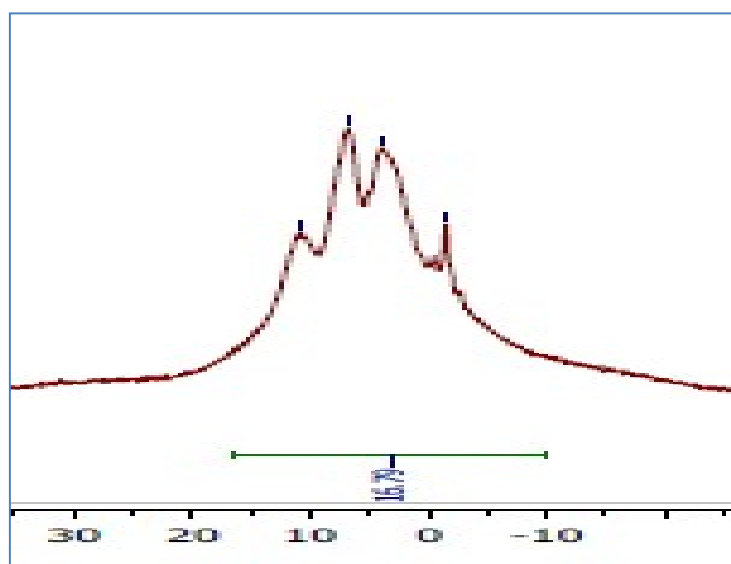


Figure S1. Reaction scheme of TNAA synthesis

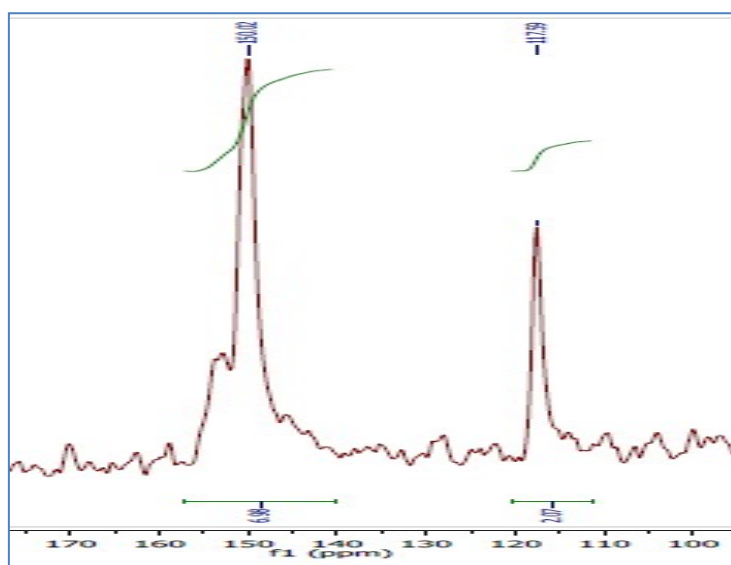
### 2. Characterization of TNAA

TNAA was characterized by thermal and spectroscopic tools in details. Elemental analysis was carried on VarioMICRO instrument. Elemental analysis (C<sub>2</sub>H<sub>2</sub>N<sub>5</sub>O<sub>9</sub>:239.06) showed C, 10.2; H, 0.86; and N, 32.74% which found to be close to reported data by Thao et. al[1]. Thermo-gravimetric analysis (TGA) analysis of TNAA was done on Q600SDT Thermal analyzer of TA Instruments. TGA of pure TNAA showed the onset at about 100°C and complete decomposition by 150°C (figure 8(b)). Fourier transform infrared spectra (FT-IR) were recorded on Nicolet iS10 spectrometer of Thermo Scientific (figure 6(c)). FTIR analysis showed strong peaks at 3419, 3385, 3269, 1690, 1641, 1602, 1533, 1477, 1390, 1352, 1300, 1171, 1064, 854, 798, 737, 642 and 577 cm<sup>-1</sup> which confirmed the functional group of TNAA.

Solid state nuclear magnetic resonance (NMR) spectrometry analysis of TNAA was considered due to its solubility and compatibility issues with various solvents.  $^1\text{H}$  and  $^{13}\text{C}$  nuclear magnetic resonance spectrometer (NMR) spectra of solid samples were recorded on Bruker MSL-300. Solid state  $^1\text{H}$  and  $^{13}\text{C}$  NMR (fig. S2(a&b)) confirmed the single hydrogen peak at 8.5 ppm and two carbon peaks at 118 (C- $\text{NO}_2$ ) and 150 (C-OH) ppm respectively.



(a)

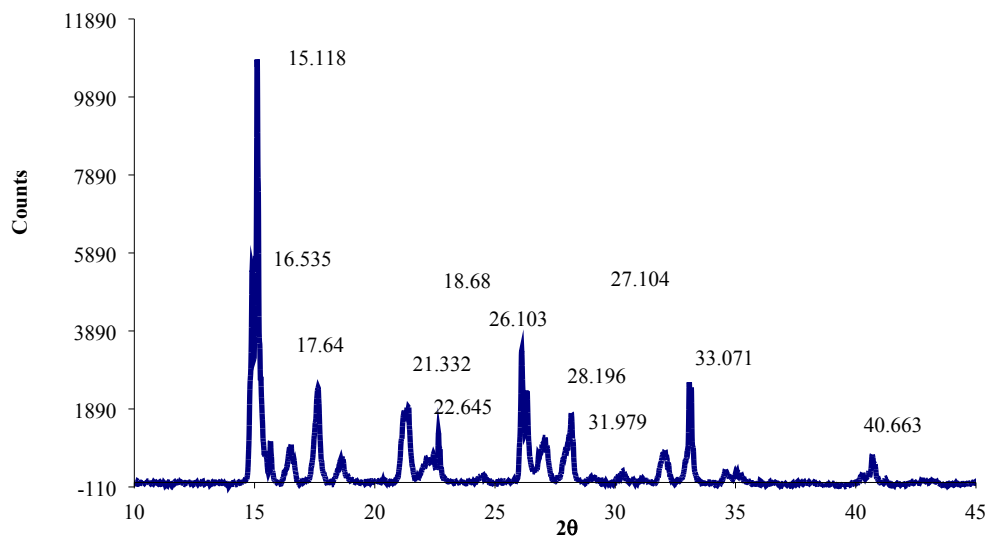


(b)

**Figure S2. (a)  $^1\text{H}$ , (b)  $^{13}\text{C}$  NMR spectra of TNAA**

The crystalline behavior of TNAA was analyzed from XRD spectra (fig. S3). X-ray diffraction was carried out on PANalytical, X-pert PRO machine equipped with

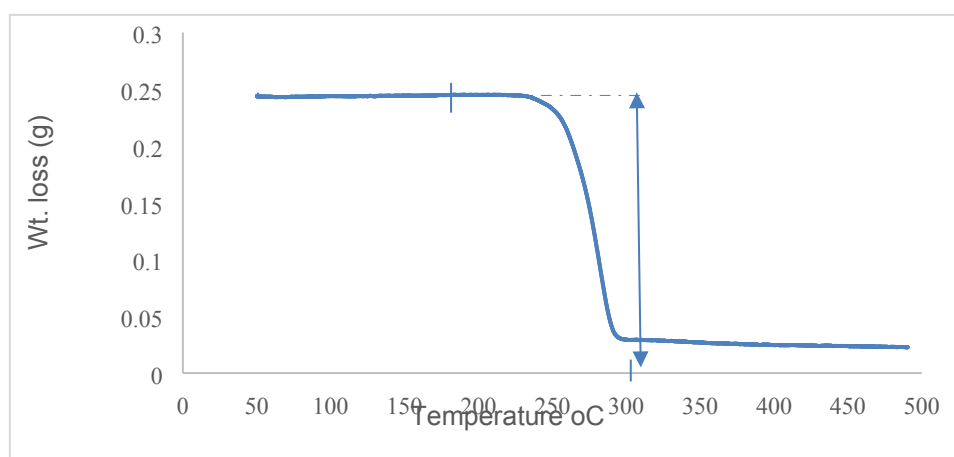
copper tube. Pattern was measured between 0 to 80° 2θ with a step width of 0.013° and a measuring time of 1s per step. The peak positions around 15.12, 17.64, 21.33, 26.1, 28.2 and 33.07 were observed in prominent manner.



**Figure S3. XRD pattern of TNA A**

### 3. TGA of compound obtained from DMF medium

Thermal analysis of compound obtained in DMF medium was carried out in DSC7 and SDTA Q600. Figure S4 shows the TGA profile of this compound.



**Figure S4. TGA of compound obtained from DMF medium**

TGA analysis shows that stability of compound obtained from DMF till 217°C. Complete decomposition of compound was noticed at about 295°C. This clearly indicates as new compound rather than TNAA.

#### 4. Reference

1. T. T. Vo, D.A. Parrish, J.n.M. Shreeve, Tetranitroacetimidic Acid: A High Oxygen Oxidizer and Potential Replacement for Ammonium Perchlorate, *J. Am. Chem. Soc.***2014**, 136(34), 11934