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Supplementary Information

Synthesis and Properties of Two Energetic Salts Based on 1-Amino-2-nitroguanidine

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Experimental Section

Safety precautions: CAUTION!!! Although none of the compounds described herein have exploded or detonated in the course of this research, these materials should be handled with extreme care by using best safety practices (leather gloves, leather coat face shield, etc.).

General procedure for the synthesis of these salts

1-amino-2-nitroguanidinum chloride, 2,4,5-trinitroimidazole and 5-nitrotetrazole were prepared according to References 1, 2 and 3, respectively.

Silver salts were prepared as follows: to a solution of 2,4,5-trinitroimidazole (2.02 g, 10 mmol), or 5-nitrotetrazole (1.14 g, 10 mmol) in water (30 mL) were added dropwise a solution of silver nitrate in water and many solids were formed immediately. Then the suspension were stirred for 2 h at room temperature and filtered, then washed with ice water. The silver salts were obtained in excellent yield.

The titled energetic salts were prepared as follows: to a suspension of the silver salts in water (30 mL) were added slowly a solution of 1-amino-2-nitroguanidinum chloride (1.55 g, 1 mmol) in water (15 mL). The resulting reaction mixture was stirred at 40 °C for 6 h and filtered. The filtrate was concentrated under reduced pressure and the collected residue was recrystallized from methanol/water to afford the corresponding product in excellent yield.

1-amino-2-nitroguanidinum 2,4,5-trinitroimidazole salt: yield: 84.6%; ^{1}H NMR (500 MHz, DMSO-d$_6$) δ_H 9.7 (s, 1H, NH), 8.4 (s, 2H, NH_2), 6.7 (s, 3H, NH_3^+); ^{13}C NMR (125 MHz, DMSO-d$_6$) δ_C 138.4, 146.9, 159.7; IR (KBr) ν_{max}/ cm^{-1} 3318, 2999, 1632, 1540, 1474, 1398, 1392, 1280, 1222, 1191, 1110, 1026, 909, 870, 834, 783, 587; ESI-MS *m/z* 202 $[M - H]^-$, 120 $[M + H]^+$; elemental analysis calcd. for $C_4H_{12}N_{18}O_8$: C 14.91, H 1.88, N 43.48; found: C 14.83, H 1.97, N 43.53.

1-amino-2-nitroguanidinum 5-nitrotetrazole salt: yield 86.1%; ^{1}H NMR (500 MHz, DMSO-d$_6$) δ_H 9.4 (s, 1H, NH), 8.4 (s, 3H, NH_3^+), 8.0 (s, 2H, NH_2); ^{13}C NMR (125 MHz, DMSO-d$_6$) δ_C 159.6, 169.2; IR (KBr) ν_{max}/ cm^{-1} 3468, 3359, 2949, 2700, 2162, 2070, 1645, 1508, 1481, 1453, 1396, 1321, 1276, 1239, 1107, 904, 834, 782, 666, 545, 486; ESI-MS *m/z* 114 $[M - H]^-$, 120 $[M + H]^+$; elemental analysis: calcd. for $C_4H_{12}N_{18}O_8$: C 10.26, H 2.58, N 59.82; found: C 10.19, H 2.62, N 59.91.

References

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2. Cho, J. R.; Kim, K. J.; Cho, S. G.; Kim, J. K.; *J. Heterocycl. Chem.*, **2002**, *39*, 141.
3. Lee, K. Y.; Coburn, M. D.; *J. Energ. Mater.* **1983**, *1*, 109.

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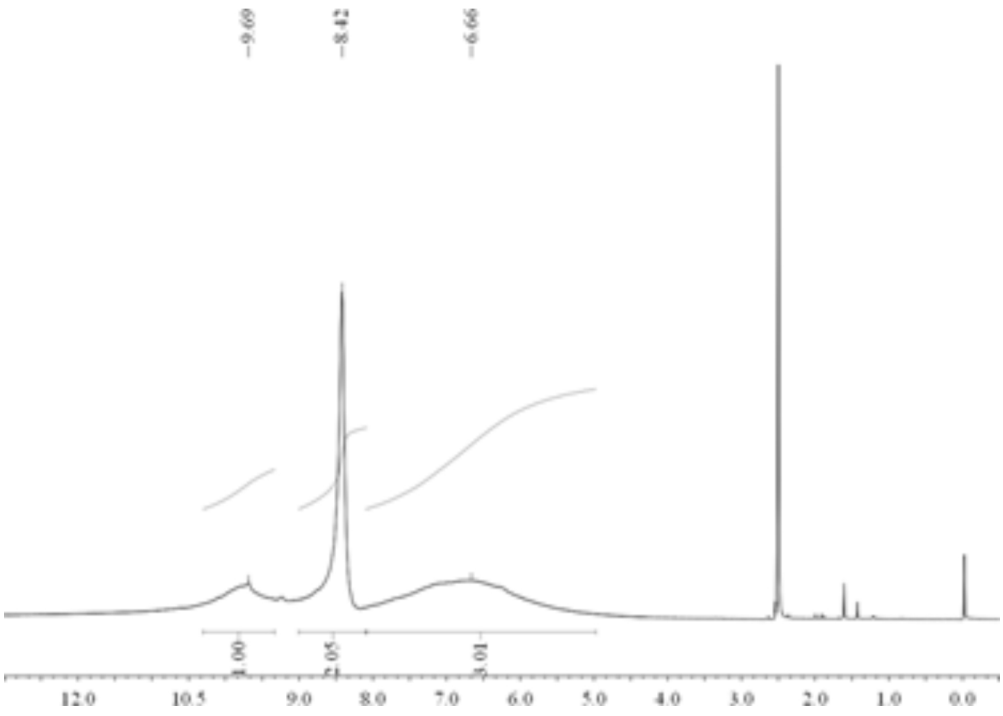

Figure S1. ^{1}H NMR spectrum (500 MHz, DMSO-d_6) of 1-amino-2-nitroguanidinum 2,4,5-trinitroimidazole salt.

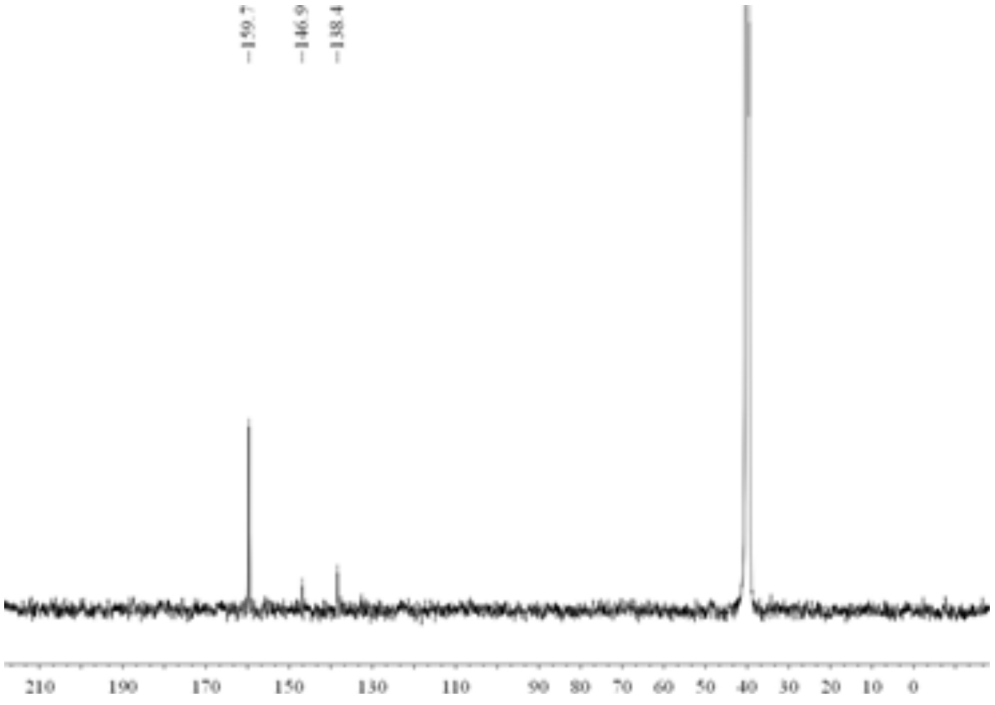

Figure S2. ^{13}C NMR spectrum (125MHz, DMSO-d_6) of 1-amino-2-nitroguanidinum 2,4,5-trinitroimidazole salt.

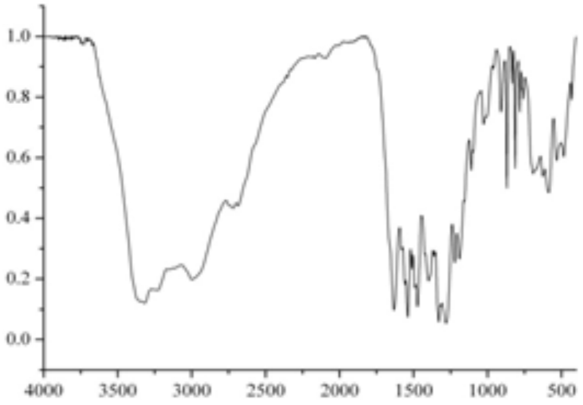

Figure S3. IR spectrum (KBr) of 1-amino-2-nitroguanidinum 2,4,5-trinitroimidazole salt.

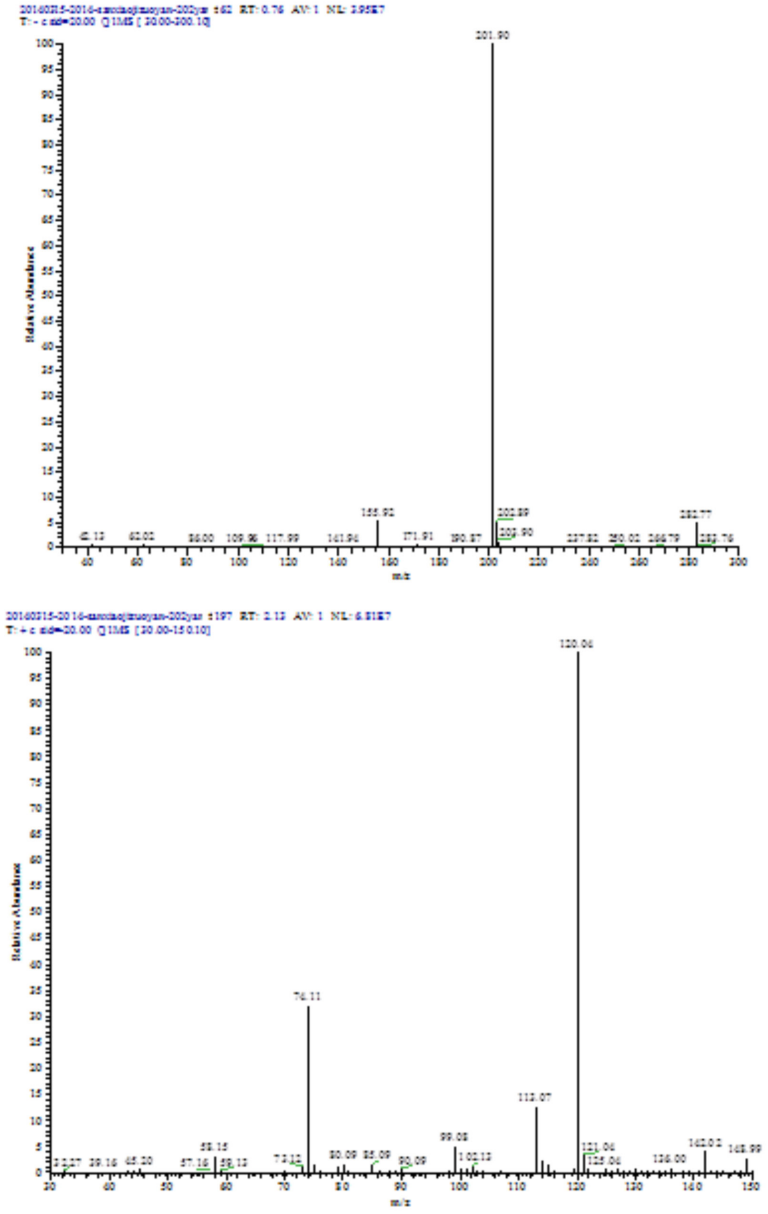

Figure S4. ESI-MS spectrum of 1-amino-2-nitroguanidinum 2,4,5-trinitroimidazole salt.

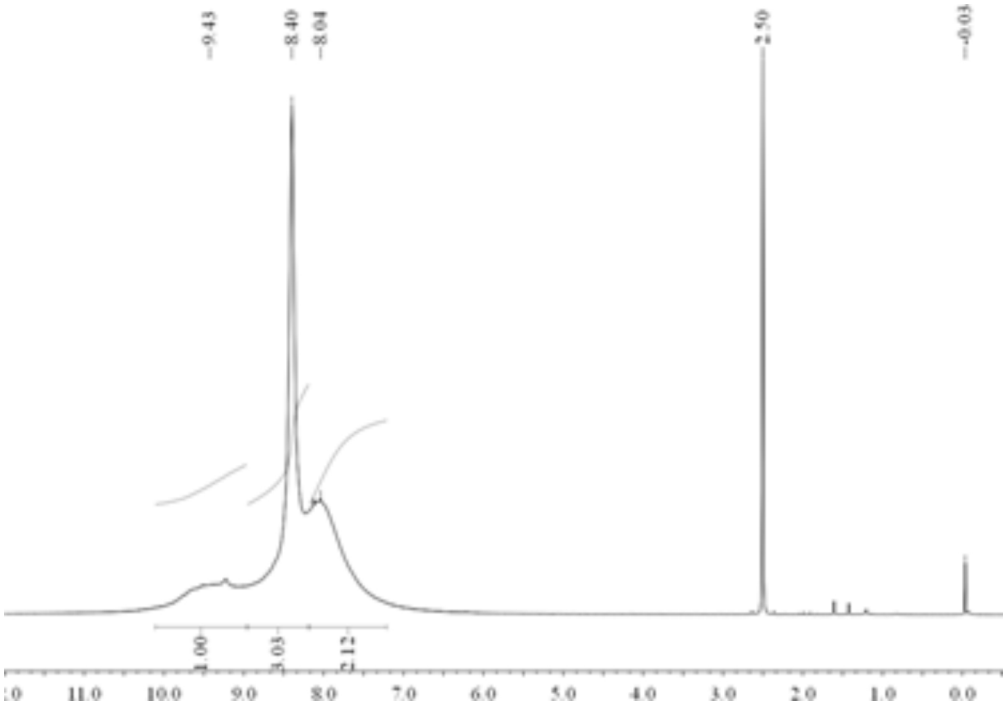

Figure S5. ^{1}H NMR spectrum (500 MHz, DMSO-d_6) of 1-amino-2-nitroguanidinum 5-nitrotetrazole salt.

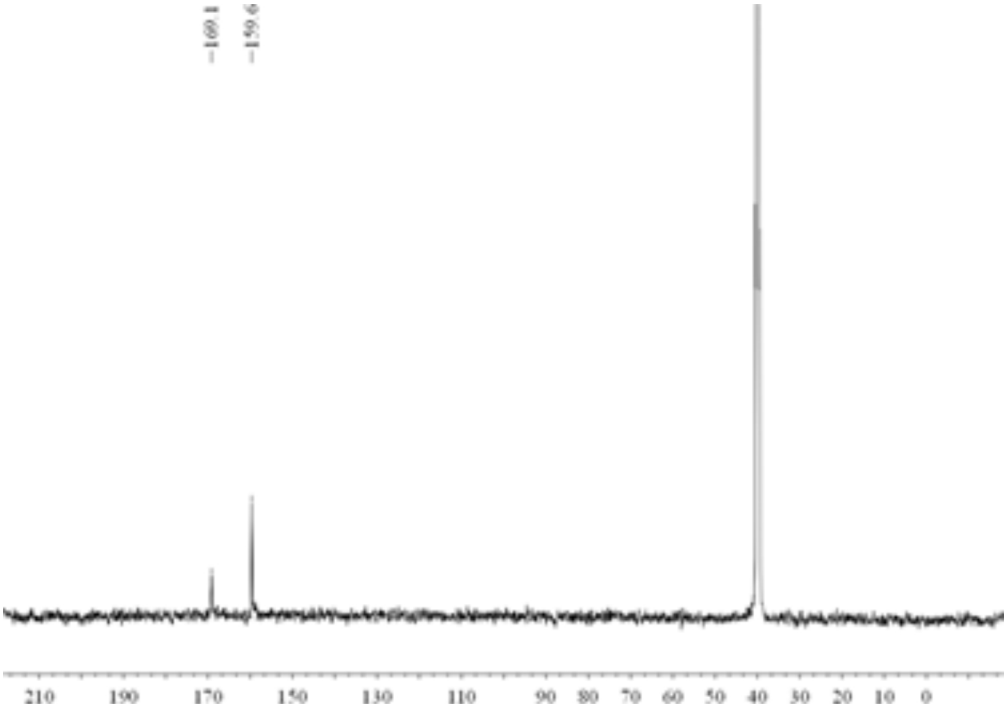

Figure S6. ^{13}C NMR spectrum (125MHz, DMSO-d_6) of 1-amino-2-nitroguanidinum 5-nitrotetrazole salt.

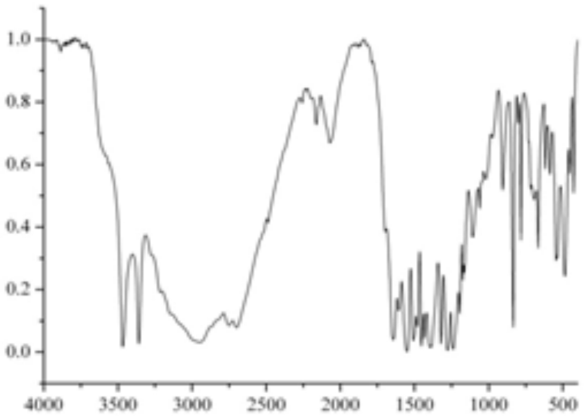

Figure S7. IR spectrum (KBr) of 1-amino-2-nitroguanidinum 5-nitrotetrazole salt.

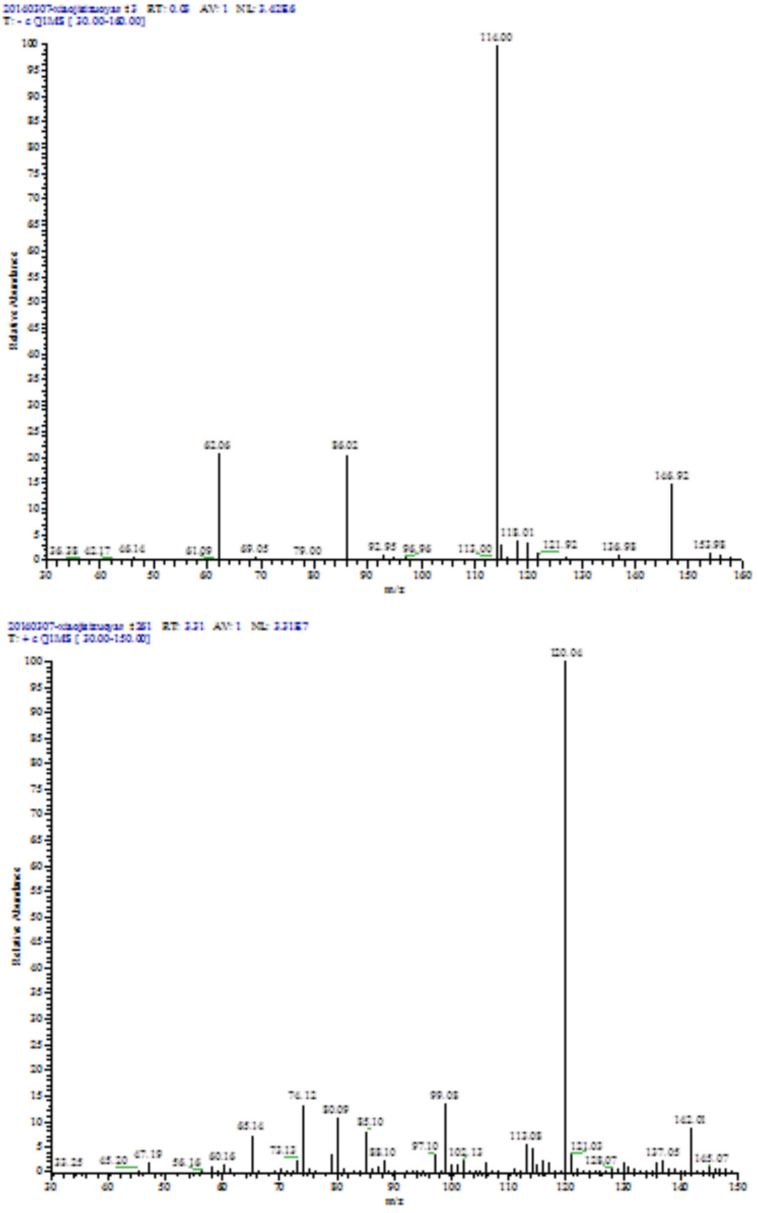

Figure S8. ESI-MS spectrum of 1-amino-2-nitroguanidinum 5-nitrotetrazole salt.