

Synthesis, Characterization and Combustion of Triazolium Based Salts

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ABSTRACT

Salts being liquid below 100 °C are defined as ionic liquids^[1]. They are receiving an increasing interest due to their unique properties and are also under investigation in the field of energetic materials. Potential applications are plasticizers, high explosives, gun and liquid rocket propellants. As a promising candidate for a high energy propellant, this paper presents the synthesis and some properties of 4-Amino-1-methyl-1,2,4-triazolium nitrate (AMTN). It has a glass transition point of -55 °C and shows good stability. Due to the very low vapor pressure a significantly reduced environmental risk, better storage and handling properties are expected. The combustion behavior was investigated in a window bomb under pressures up to 15 MPa resulting in a linear burning characteristic with low pressure dependence. Moreover, 4-Amino-1-methyl-1,2,4-triazolium perchlorate (AMTP) was synthesized and characterized. With its melting point close to TNT, AMTP has potential as a melt cast explosive. The enthalpy of formation was determined and the predicted performance was compared with TNT. For comparison the 4-Amino-1-H-1,2,4-triazolium salts were also synthesized.

INTRODUCTION

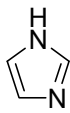
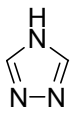
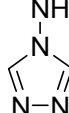
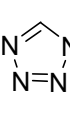
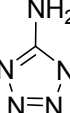
Ionic liquids (ILs) are in the focus of recent research and finding application in more and more fields of life. The applications range from novel reaction media^[2], as electrolytes in batteries^[3], solar cells^[4], gas storing media^[5], lubricants^[6] and heat transfer fluids^[7], to mention only a small excerpt of the investigated and in use applications. The research on ILs began already in 1888 with ethanolanmonium nitrate ($T_m = 52\text{-}54\text{ }^{\circ}\text{C}$), an energetic protic IL synthesized and characterized by Gabriel^[8] and continued with ethylammonium nitrate ($T_m = 13\text{-}14\text{ }^{\circ}\text{C}$; Paul Walden

1914^[9]). However, the new class of ionic liquids only became subject of interest in the late 1990s were the publications on ILs started growing exponentially.

In general protic ionic liquids are formed by proton transfer between Brønsted acids and bases, whereas aprotic ILs are usually synthesized through S_N2 alkylation reactions and subsequent anion metathesis.

The properties attributed to aprotic ionic liquids are good thermal stability, very low vapor pressure, electric conductivity, good solvent power and a high heat capacity. Shreeve et al.^[10] had investigated a series of new energetic ionic liquids (EILs) but there is still a big undiscovered field due to the great number of possible combinations of energetic anions and cations. Thermal analysis revealed that protonated salts exhibit a significantly lower stability than those of alkylated derivatives^[11]. An overview of possible starting materials for EILs is given in Table 1. One has to take into account that 4-Amino-1,2,4-triazole has to be alkylated only once to yield a cation while the other listed heterocycles have to be alkylated twice to produce a cation. The structure isomer of 4-AT, 1-Amino-1,2,3-triazole is also an interesting starting material missing in the overview. However, EILs based on 1-Amino-1,2,3-triazole have much higher melting or glass transition points.

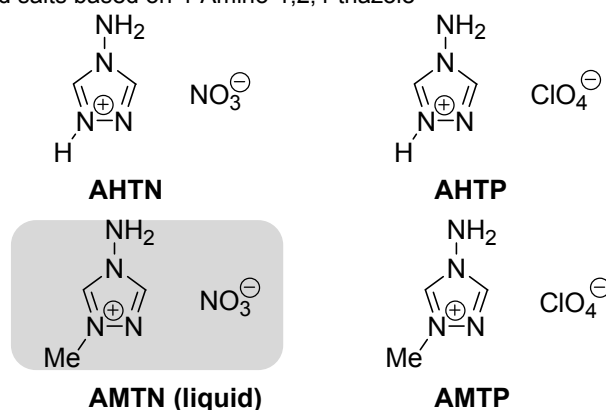
Table 1: Overview of some possible starting materials for EILs^[12].

						
$\Delta_f H_m^\circ$	[kJ/mol]	+49.8 ^[12a]	+108.7 ^[12c]	+318.0 ^[12a,c] +222.8 ^[12b] +223.5	+236.0 ^[12a]	209.2 ^[12a]
OB	[%]	-188.0	-127.4	-114.2	-68.5	-65.8
T _{dec}	[°C]	> 257 ^[12a]	> 260 ^[12a]	270 ^[12a]	188 ^[12d]	≥ 206 ^[12e]

The enthalpy of formation ($\Delta_f H_m^\circ$) of 4-Amino-1,2,4-triazole (4-AT) commonly referenced in the literature as +318.0 kJ/mol appears to be too high. More recently a new value was published (+222.8 ± 1.8 kJ/mol), which is in good agreement with the theoretical prediction.

To verify this value, some measurements in the calorimetric bomb were performed and resulted in an enthalpy of formation of +223.5 ± 2 kJ/mol, taking into account the formation of nitric acid. The synthesized compounds shown in Table 2 were first mentioned and only partly described in literature by Greg W. Drake et al.^[13].

Table 2: Synthesized salts based on 4-Amino-1,2,4-triazole



RESULTS AND DISCUSSION

In ionic liquids even small amounts of impurities (water, solvents or other ions) change the physiochemical properties significantly, which can be seen on literature data. For example the enthalpy of formation of AMTN is published with three different values: -187 kJ/mol^[14], +58 kJ/mol^[15] and a theoretical value of -27.6 kJ/mol^[16]. An overview of the physicochemical properties of the synthesized compounds is shown in Table 3.

Table 3: Properties of the synthesized compounds.

			AHTP	AMTP	AHTN	AMTN
T _g	[°C]		-	-	-	-55
T _m	[°C]		83	84	67	-
T _{dec}	DSC	[°C]	291	290	229	259
	TGA	[°C]	294	274	207	246
Density	[g/cm ³]		1.85 ^[b]	1.64 ^[b]	1.63 ^[b]	1.44
Nitrogen content	[%]		30.36	28.22	47.61	43.47
Impact	[Nm]		5	7.5	> 60	15
Friction	[N]		18	64	> 360	144
Oxygen balance	[%]		-21.7	-44.3	-38.1	-64.5
Decomposition enthalpy DSC ^[a]	[J/g]		6056	5602	2635	2628

[a] measured in gold-plated and pressure-sealed pans. [b] density of powdered material.

A fast method revealing the overall purity of EILs is achieved by cyclic voltammetry. The cyclic voltammogram of AMTN measured against gold electrodes is shown in Figure 1 resulting in an electrochemical window of 3 Volts.

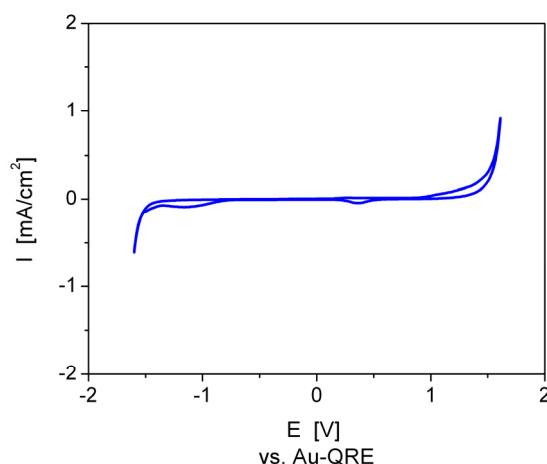


Figure 1: Cyclic voltammogram of AMTN measured against Au-QRE.

The compounds 4-Amino-1-H-1,2,4-triazolium perchlorate / nitrate (AMTP / AMTN) were synthesized by simple proton transfer between perchloric / nitric acid and 4-AT resulting in hygroscopic salts. The protonated perchlorate salt may not be useable for practical applications because of its high mechanical sensitivity (18 N) combined with its strong respond (probably detonation) upon friction stimuli resulting in scattering the ceramic friction plate. It was suggested as a TNT replacement in combination with lithium nitrate or other salts approaching the energy output of RDX^[17, 18]. On the other hand the analogous nitrate salt is very

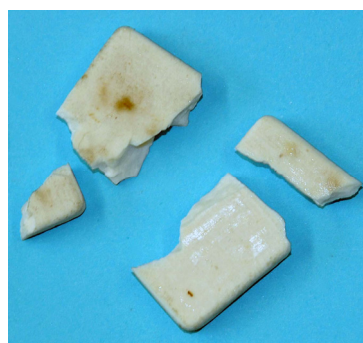


Figure 2: Ceramic plate scattered by AHTP during friction test.

insensitive and much more favorable as an ingredient in melt cast explosive formulations together with other energetic salts to adjust the melting point. AMTN was tested as a phase stabilizing additive in ammonium nitrate up to 5 wt%. However, the AHTN / AN mixtures still showed polymorphic phase transitions below 60 °C.

Instead of protonating 4-AT to produce salts or ionic liquids, methylation in N1 position will decrease the performance and oxygen balance but stability and compatibility will be increased considerably. In addition, hygroscopicity is reduced drastically which is very important for practical applications.

Methylation of 4-AT, which contains two C-H linkages in the ring as well as a pendant NH₂ group, performs selectively in the N1 position and breaks the mirror symmetry of the ring. This can be seen in the proton spectra by the disappearance of the singlet derived from the two C-H protons and the appearance of two equal downfield C-H singlets. A similar effect can be seen in the ¹³C-NMR upon

quaternisation of compound 4-AT, which also resulted in two singlets. The infrared spectra (top) and RAMAN spectra (bottom) of AMTN and AMTP are shown in Figure 3. The most intense bands in the Raman spectra for AMTN is associated with the nitrate anion around 1044 cm^{-1} , while in the infrared spectra strong stretches centered at 1318 cm^{-1} ^[19]. The spectra AMTP is dominated by the powerful bands of the perchlorate anion; in the infrared, strong bands centered at 1071 cm^{-1} , while in the Raman, strong bands appear at 933 cm^{-1} and 462 cm^{-1} . These have been also observed previously in several other perchlorate salt systems^[20].

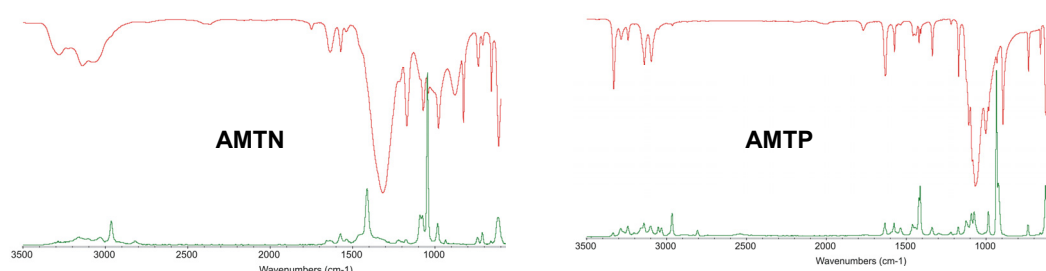


Figure 3: IR (top) and RAMAN (bottom) spectra of AMTN and AMTP.

AMTP has a melting point of $84\text{ }^{\circ}\text{C}$ which is close to TNT ($80.8\text{ }^{\circ}\text{C}$ ^[21]). From this point of view it has potential as a melt cast explosive with increased performance (VOD's: AMTP = 7287 m/s versus TNT = 6886 m/s); see Table 4. This application together with the advantage of a very low vapor pressure was recently published as a patent^[17]. However, in terms of current demands regarding insensitivity – the friction sensitivity of AMTP of 64 N is far too sensitive for applications in modern insensitive energetic materials. Batches with different crystal sizes and melt cast samples delivered all similar sensitivity results.

AMTN is an energetic ionic liquid (EIL) fitting the practical demands with a glass transition point of $-55\text{ }^{\circ}\text{C}$ and a thermal stability of above $200\text{ }^{\circ}\text{C}$. Because of the asymmetrical triazolium cation and the symmetrical nitrate anion an efficient crystal packing is inhibited. A theoretical explanation for the low melting or glass transition points of ILs is based on the free Gibbs energy of fusion. The liquid state in ILs is thermodynamically favorable, because of the size and conformational flexibility of the ions involved, resulting in small lattice enthalpies and large entropy changes that favor melting^[22].

EILs have a broad potential field of applications and even give access to new energetic applications which were not possible with conventional energetic liquids due to their much higher vapor pressure and smaller operation temperature range. Because of the very low vapor pressure of EILs a significantly reduced environmental risk, better storage and handling properties are expected. In the field of energetic materials, some of the potential applications among several others are the use as energetic plasticizers or liquid missile and gun propellants. Common ionic liquids can be tailored to dissolve cellulose or wood – a challenging task in the past, where only CS_2 or other toxic and hazardous solvents could be used. Therefore dissolving or gelatinizing of nitrocellulose (NC) is also expected for ionic liquids. In order to be competitive with in terms of energy content, EILs should be used. AMTN was used to gelatinize NC (nitrogen content 12.6%) and some preliminary results are shown in Figure 4. The Figure 4a on the left is showing a microscopic picture with gelatinized NC on the left side and pure NC on the right side. Picture 4b shows a small piece of the thin foil of the gelatinized NC and at Figure 4c the foil covers a print of our institute label to document the transparency of the product.

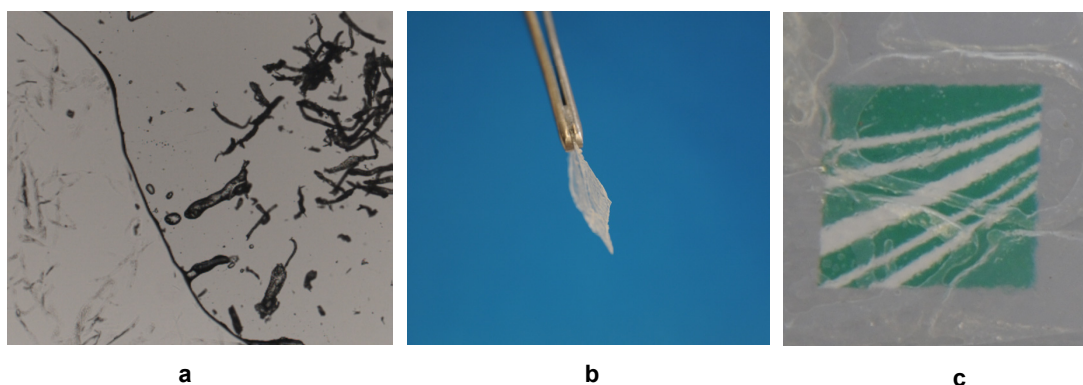


Figure 4: Gelatinization of nitrocellulose (N = 12.6%) with AMTN.

One has to take into account that for common nitrate esters like nitroglycerine, a much higher content of plasticizer is needed to achieve transparent foils with nitrocellulose, whereas for AMTN ratios starting from 4:1 (by weight) are already sufficient to produce transparent foils. To our knowledge this is the first published example of the gelatinizing ability of EILs for NC

First burning tests of AMTN were conducted in atmospheric air, putting single drops inside a DSC aluminum pan of 5 mm diameter. Ignition was performed using a blowtorch. As shown in Figure 5a reproducible and stable burning flame developed, increasing drastically in volume when the sample heats up. A flame

temperature of 2100 to 2200 K was measured by analyzing NIR-emission spectra according to a method described elsewhere ^[23].

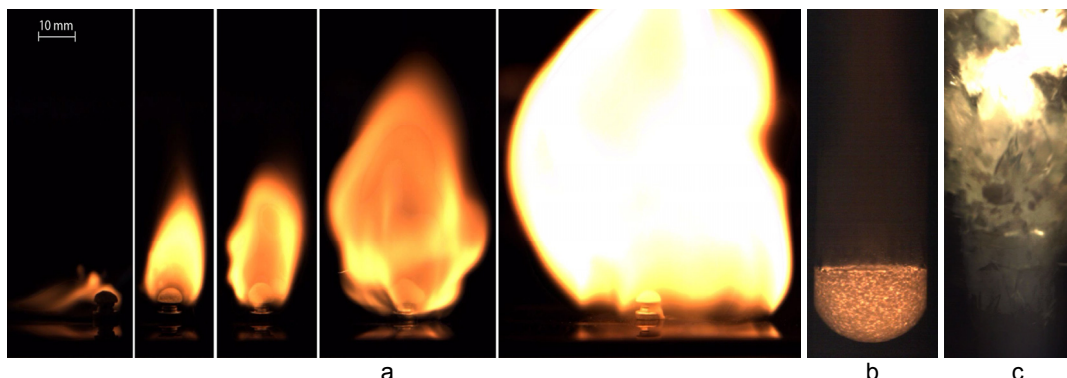


Figure 5: Burning of AMTN in atmospheric air (a), under nitrogen (b) and deflagration of AMTP (c).

An equimolar mixture of AMTN and 4-AT (1:1 mol) also forms a liquid ($T_g = -59\text{ }^{\circ}\text{C}$) which might be useful as an energetic fuel because of the high enthalpy of formation of 4-AT. Moreover, due to the unique solubility abilities of ionic liquids a variety of common energetic substances can be dissolved for improving and tuning the performance in the desired field of application.

Samples were filled into glass test tubes (\varnothing 8 mm) and burnt in analogy to solid propellant strands in a window bomb under nitrogen at pressures up to 15 MPa at room temperature. Soon after ignition using a melting wire a stable combustion developed with a distinct, intensively emitting reaction inside the condensed phase. Above a weak glowing flame could be observed (Figure 5b).

The tests resulted in a strongly linear regression as shown in Figure 6. The burning rates of the investigated liquids were in the range of 6–50 mm/s. Burning rate did not strongly increase with pressure like classic liquids or solid propellants. Pure AMTN showed only at pressures above 13 MPa a reproducible burning. An eutectic mixture of AMTN / AMTP (94 / 6 wt%) showed significantly higher burning rates up to 50 mm/s. Pure AMTP deflagrates without formation of an constant regression rate when investigated in the optical bomb under nitrogen (Figure 5c) up to 13 MPa. Even the fuel mixture AMTN / 4-ATP, despite its strongly negative oxygen balance (-81.6 %), was ignitable at lower pressures down to 4 MPa and developed a steady burning rate.

The fuel mixture AMTN / 4-AT features solid intermediary decomposition products floating on the liquid surface. Above a very weak flame zone appears. At the wall of the test tube black, probably carbonized residues were left because of the highly negative oxygen balance of the fuel rich mixture.

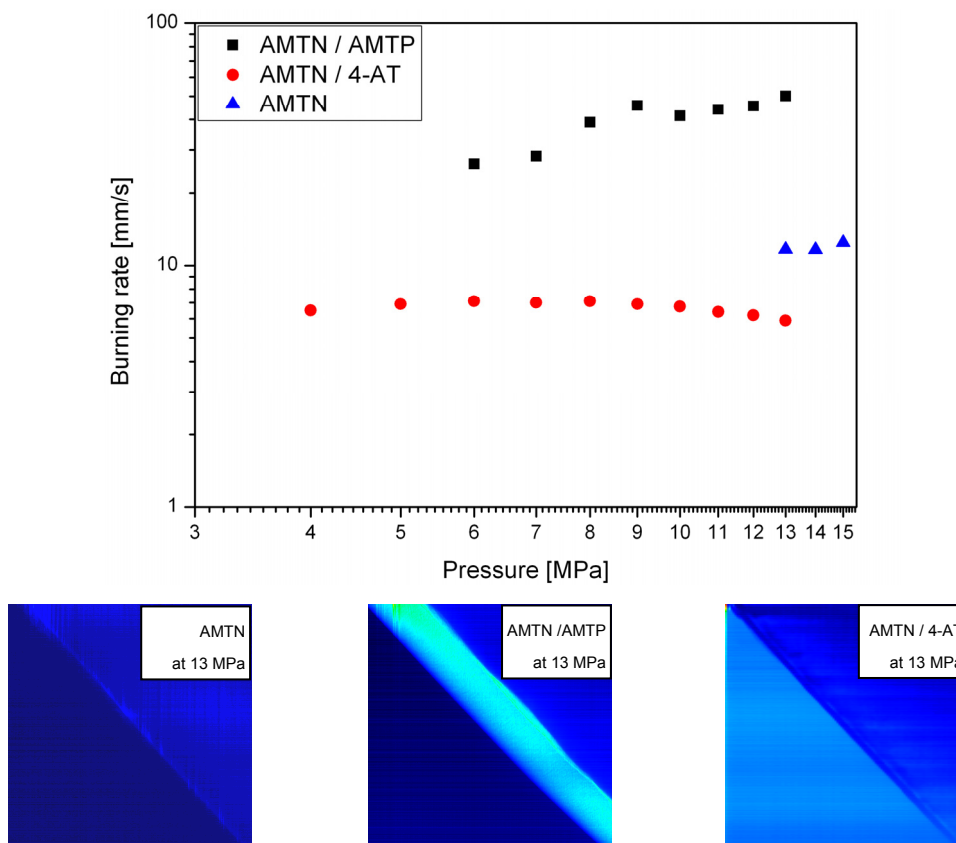
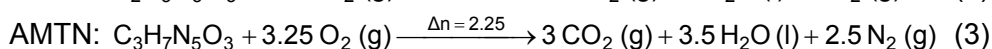
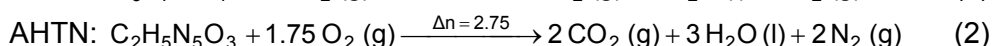
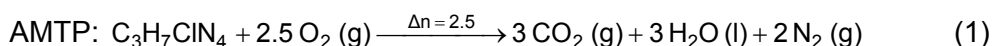


Figure 6: Burning rate evolution for pure AMTN and mixtures with AMTP and 4-AT at pressure of 4 to 15 MPa.

Due to the very low vapor pressure of ionic liquids the combustion behavior should not be controlled by evaporation like common energetic liquids but by decomposition inside the condensed phase close to the interface to the gaseous phase (Figure 5b). This reaction might be less pressure sensitive and could be the key to explain the low pressure dependency of the burning rate and will be in focus of further investigations.

To estimate the potential performance of the synthesized compounds, measurements in a calorimetric bomb were done for AMTP, AHTM and AMTN. The standard molar enthalpy of combustion ($\Delta_c H_m$) was calculated by using equation 4 with $\sum n_i$ (equation 5) as the total molar amount of gases in the products or reactants.



$$\Delta_c H_m = \Delta_c U + \Delta n RT \quad (4)$$

$$\Delta n = \sum n_i [\text{products} (\text{g})] - \sum n_i [\text{reactants} (\text{g})] \quad (5)$$

$$\Delta_f H_m^\circ (\text{C}_a\text{H}_b\text{N}_c\text{O}_d\text{Cl}_e) = a \Delta_f H_m^\circ (\text{CO}_2) + b/2 \Delta_f H_m^\circ (\text{H}_2\text{O}) + e \Delta_f H_m^\circ (\text{HCl}) - \Delta_c H_m (\text{C}_a\text{H}_b\text{N}_c\text{O}_d\text{Cl}_e) \quad (6)$$

The standard enthalpy of formation ($\Delta_f H_m^\circ$) was calculated using Hess's Law and the standard values of heats of formation for water and carbon dioxide^[24]. The formation of nitric acid was determined with ion chromatography and considered in the calculations.

Table 4: Thermochemical properties of TNT, AMTP, AHTN and AMTN.

		TNT	AMTP	AHTN	AMTN
State of matter		solid	solid	solid	liquid
Oxygen balance	[%]	-73.9	-44.3	-38.1	-64.5
$\Delta_f H_m^\circ$	[kJ/mol]	-67	+72 ± 18	+2 ± 7	-23 ± 10
Heat of explosion ^[a]	[J/g]	3766	4096	3752	3120
Gas volume (25°C) ^[b]	[mL/g]	830	1034	962	1049
Shock velocity ^[c]	[m/s]	6886	7287	7771	7056

[a] calculated with ICT Code^[25] water liquid. [b] without water. [c] calculated with CHEETAH 2.0.

Energetic ionic liquids might be useful as monopropellants for tactical missiles. To evaluate its potential, the volume specific impulse of AMTN was calculated with the ICT code^[25] and compared to traditional monopropellants like nitromethane and isopropylnitrate. In Figure 7 the volume specific impulse (equilibrium flow) calculated with the ICT code is shown.

Table 5: Physical properties of nitromethane, isopropylnitrate^[26] and AMTN.

	Melting point	Boiling point	Density	Vapor pressure (at 298 K)
	[°C]	[°C]	[g/cm ³]	[kPa]
Nitromethane	-28	101	1.14	4.8
Isopropylnitrate	-82	100	1.03	3.5
AMTN	-55	(T _{dec} > 200)	1.44	< 0.001

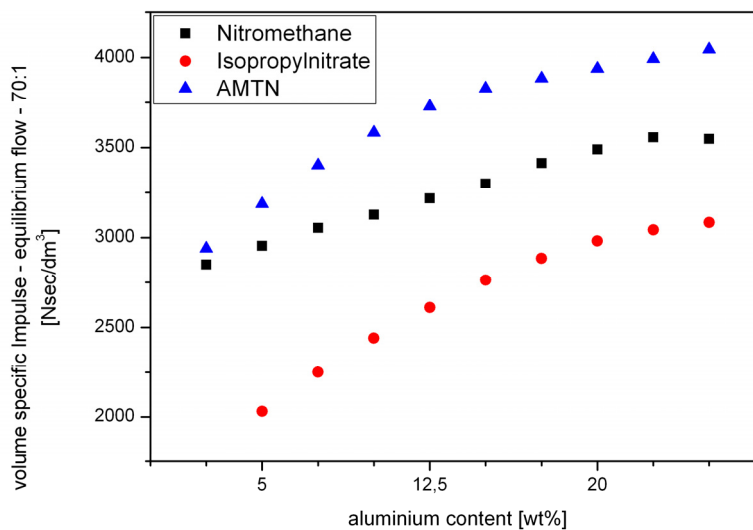


Figure 7: Volume specific impulse (equilibrium flow) of nitromethane, isopropylnitrate and AMTN with increasing aluminium content at an expansion ratio of 70:1.

The volume specific impulse of AMTN with aluminum is outranging the monopropellants nitromethane and isopropylnitrate, allowing new small and powerful missiles.

EXPERIMENTAL

^1H -NMR and ^{13}C -NMR were conducted on a 400 MHz Bruker AV-400 spectrometer in $\text{DMSO-}d_6$. Differential scanning calorimetry (DSC) was done by a TA instruments Q 1000 using pierced aluminum pans. Scans were carried out on each sample, at scan rates of $5\text{ }^\circ\text{C/min}$, under argon flux. The reported values are onset temperatures. Glass transition points were measured from the 2nd heating cycle after cooling to $-90\text{ }^\circ\text{C}$. Decomposition enthalpy was measured on a TA instruments MDSC 2920 using gold-plated and pressure-sealed pans. Thermogravimetric analysis (TGA) was done by a TA Q500 apparatus with a scan rate of $5\text{ }^\circ\text{C/min}$ under nitrogen flux. Reported values are the central points according to DIN EN ISO 11358. Infrared spectroscopy was done on a Nicolet SX 5 spectrometer and Raman spectroscopy on a Bruker RFS 100/S (Nd:YAG laser 1064 nm). Density was measured with a PYCNOMATIC ATC from Thermo Electron Corporation, ion analysis with a DIONEX ICS-3000 and elementary analysis with a FLASH EA 1112 Series from Thermo Electron Corporation. For all calorimetric measurements, an IKA C 2000 system was used. The calorimetric bomb was filled in each case with 5 mL water (HPLC purity) and after each run the combustion products were examined for unburned carbon. The combustion experiment was repeated four times and nitric acid formation was determined by measuring the nitrate content in the water after each run. Reported values are the average of four measurements. Cyclic voltammetry was measured using $10\text{ }\mu\text{L}$ of an EIL and gold micro electrodes (active radius = $50\text{ }\mu\text{m}$, 20 mV/sec). Impact sensitivity and friction sensitivity tests were determined according to NATO STANAG 4487 and NATO STANAG 4489 procedures with the BAM drop hammer and friction sensitivity tester made by the former company Julius Peter (Berlin). The value reported is the smallest load under which deflagration has been noticed at least one time in six consecutive tests. Residual silver analyses were carried out on a Thermo Scientific iCAP 6300 ICP and all synthesized samples after purification having a silver content of below 100 ppm . All chemical reagents and solvents of analytical grade were obtained from Sigma–Aldrich, ROTH and Merck and used as supplied. 4-Amino-1-H-1,2,4-triazolium nitrate (AHTN) and 4-Amino-1-H-1,2,4-triazolium perchlorate (AHTP) were prepared according to literature procedures^[18].

4-Amino-1-methyl-1,2,4-triazolium iodide (AMTI)

To a solution of 4-Amino-1,2,4-triazole (4-AT) (159.75 g, 1.90 mol) in 200 mL DMSO and 250 mL MeCN, 124.5 mL iodomethane (283.88 g, 2.00 mol) was added gradually and stirred at 30 °C in the dark for 3 days. Upon addition of n-propanol AMTI crystallized in the cold and was recrystallized twice from isopropanol, yielding white needles 352 g (82 %). mp 99.0 °C. IR (cm⁻¹) ν : 3215, 3118, 3002, 1608, 1566, 1444, 1405, 1331, 1170, 1067, 972, 866, 731. Raman (cm⁻¹) ν : 3141, 3012, 2919, 2806, 1612, 1568, 1407, 1332, 1171, 1089, 1068, 978, 860, 666, 617, 456. ¹H NMR (400.13 MHz, DMSO-*d*₆) δ : 4.03 (s, 3H, N1-Me), 6.95 (s, 2H, NH₂), 9.16 (s, 1H, C3), 10.10 (s, 1H, C5) ppm. ¹³C NMR (100.62 MHz, DMSO-*d*₆) δ : 38.8 (Me), 142.8 (C3), 145.0 (C5) ppm. Elemental analysis calcd (%) for C₃H₇N₄: C 15.94, H 3.12, N 24.79; found: C 15.97, H 3.04, N 24.93.

4-Amino-1-methyl-1,2,4-triazolium nitrate (AMTN)

To a magnetically stirred solution of 4-Amino-1-methyl-1,2,4-triazolium iodide (AMTI) (113.010 g, 0.50 mol) in methanol (600 mL) was added drop wise a solution of silver nitrate (AgNO₃, 84.935 g, 0.50 mol) in 40 mL HPLC water. After stirring 12 h in the darkness at room temperature, the insoluble silver iodide was removed by filtration through layers of Celite and sea sand. Then the solvents were evaporated and the liquid was stirred under high vacuum at 60 °C for 12 h and stored for one week over P₂O₅ in high vacuum yielding AMTN as colorless oil (75.20 g, 93 %). T_g = -55 °C, T_{dec} = 262 °C. IR (cm⁻¹) ν : 3282, 3141, 3079, 2393, 1750, 1637, 1573, 1537, 1317, 1171, 1071, 979, 881, 828, 658. Raman (cm⁻¹) ν : 3155, 2963, 1574, 1410, 1089, 1074, 1044, 981, 934, 740, 711, 616, 457, 313, 98. ¹H NMR (400.13 MHz, DMSO-*d*₆) δ : 4.04 (s, 3H, N1-Me), 6.96 (s, 2H, NH₂), 9.11 (s, 1H, C3), 10.12 (s, 1H, C5) ppm. ¹³C NMR (100.62 MHz, DMSO-*d*₆) δ : 39.0 (Me), 143.3 (C3), 145.3 (C5) ppm. Elemental analysis calcd (%) for C₃H₇N₅O₃: C 22.69, H 4.38, N 43.34; found: C 22.24, H 4.28, N 43.35.

4-Amino-1-methyl-1,2,4-triazolium perchlorate (AMTP)

To a magnetically stirred solution of 4-Amino-1-methyl-1,2,4-triazolium iodide (AMTI) (113.010 g, 0.50 mol) in methanol (600 mL) was added silver perchlorate (AgClO₄, 103.660 g, 0.50 mol) in 50 mL HPLC water. After 12 h in the darkness at room temperature, the insoluble silver iodide was removed by filtration through layers of Celite and sea sand and the solution was evaporated. The residue was

recrystallized twice from ethanol yielding white crystals. (88.37 g, 89 %). $T_m = 84$ °C, $T_{dec} = 290$ °C. IR (cm^{-1}) ν : 3282, 3141, 3079, 2393, 1750, 1637, 1573, 1537, 1317, 1171, 1071, 979, 881, 828, 658. Raman (cm^{-1}) ν : 3289, 3242, 3100, 2965, 1632, 1576, 1411, 1338, 1091, 1073, 984, 933, 921, 736, 627, 605, 462, 124. ^1H NMR (400.13 MHz, $\text{DMSO}-d_6$) δ : 4.04 (s, 3H, N1-Me), 6.96 (s, 2H, NH_2), 9.11 (s, 1H, C3), 10.12 (s, 1H, C5) ppm. ^{13}C NMR (100.62 MHz, $\text{DMSO}-d_6$) δ : 39.0 (Me), 143.3 (C3), 145.3 (C5) ppm. Elemental analysis calcd (%) for $\text{C}_3\text{H}_7\text{ClN}_4\text{O}_4$: C 18.15, H 3.55, N 28.22; found: C 18.22, H 3.43, N 28.37.

CONCLUSION

4-Amino-1-methyl-1,2,4-triazolium nitrate (AMTN) and perchlorate (AMTP) and its protonated analogs were successfully synthesized and characterized. The energetic ionic liquid AMTN has a glass transition point of -55 °C and shows good stability offering an increased operation temperature range. Furthermore mixtures of AMTN with nitrocellulose gelatinized and gave transparent foils. In combustion experiments AMTN and AMTP were studied. AMTN might be a valuable candidate as an energetic plasticizer or liquid rocket and gun propellant. Because of the unique properties of EILs this class of energetic materials offers a wide spectrum of possible future applications.

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ABBREVIATIONS AND SYMBOLS

$\Delta_c U$	Combustion energy
$\Delta_c H_m$	Molar enthalpy of combustion
$\Delta_f H_m^\circ$	Standard enthalpy of formation
bp	Boiling point
D	Detonation velocity
DSC	Differential scanning calorimetry
DMSO	Dimethyl sulfoxide
EIL	Energetic ionic liquid
HPLC	High pressure liquid chromatography
IC	Ion chromatography
IL	Ionic liquid
IR	Infrared spectroscopy

MeCN	Acetonitrile
MeOH	Methanol
NC	Nitrocellulose
NMR	Nuclear magnetic resonance
OB	Oxygen balance
P ₂ O ₅	Phosphorus pentoxide
ppm	Parts per million
QRE	Quasi reference electrode
T _g	Glass transition temperature
T _m	Melting point
T _{dec}	Decomposition temperature
TGA	Thermogravimetric analysis
VOD	Velocity of detonation

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