Synthesis, Characterization and Combustion of Triazolium Based Salts

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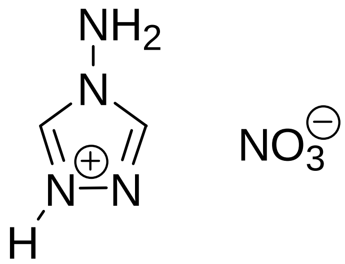
outline

- synthesized triazolium salts
- definition of Ionic Liquids
- history and development of Ionic Liquids
- results and potential applications
- summary and conclusions

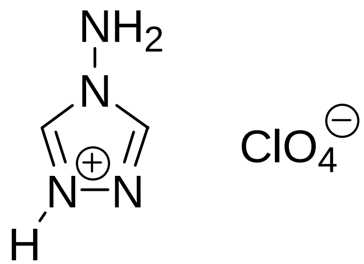
synthesized triazolium salts

- protic and aprotic triazolium salts

protonated

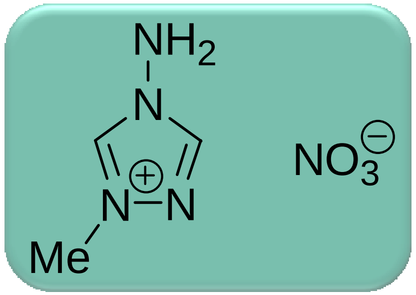


AHTN

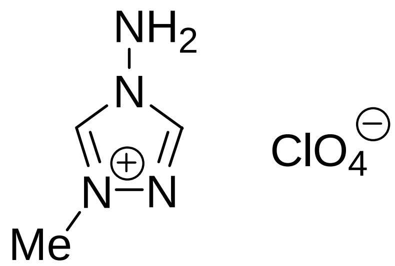


AHTP

methylated



AMTN



AMTP

liquid at room temperature

AMTN: first mentioned in literature 2002 by Greg W. Drake

definition Ionic Liquids (ILs)

cation

+

anion

- consisting entirely of cations and anions
- without molecular solvent
- mp: < 100 °C (definition)

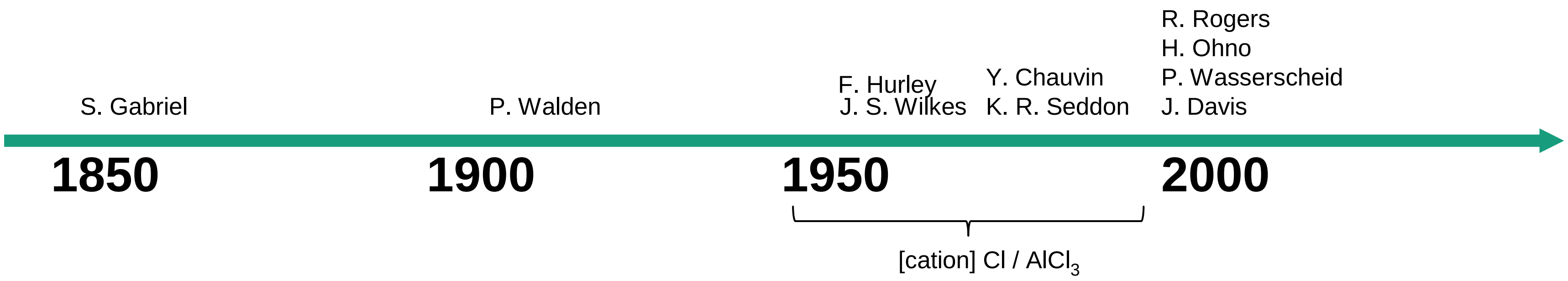
attributed properties:

- electric conductivity
- thermal stability
- very low vapor pressure
- good solvent abilities
- high heat capacity

history

first Ionic Liquids (IL):

- 1888 ethanolammonium nitrate mp: 52-55 ℃ S. Gabriel
- 1914 ethylammonium nitrate mp: 13-14 ℃ P. Walden

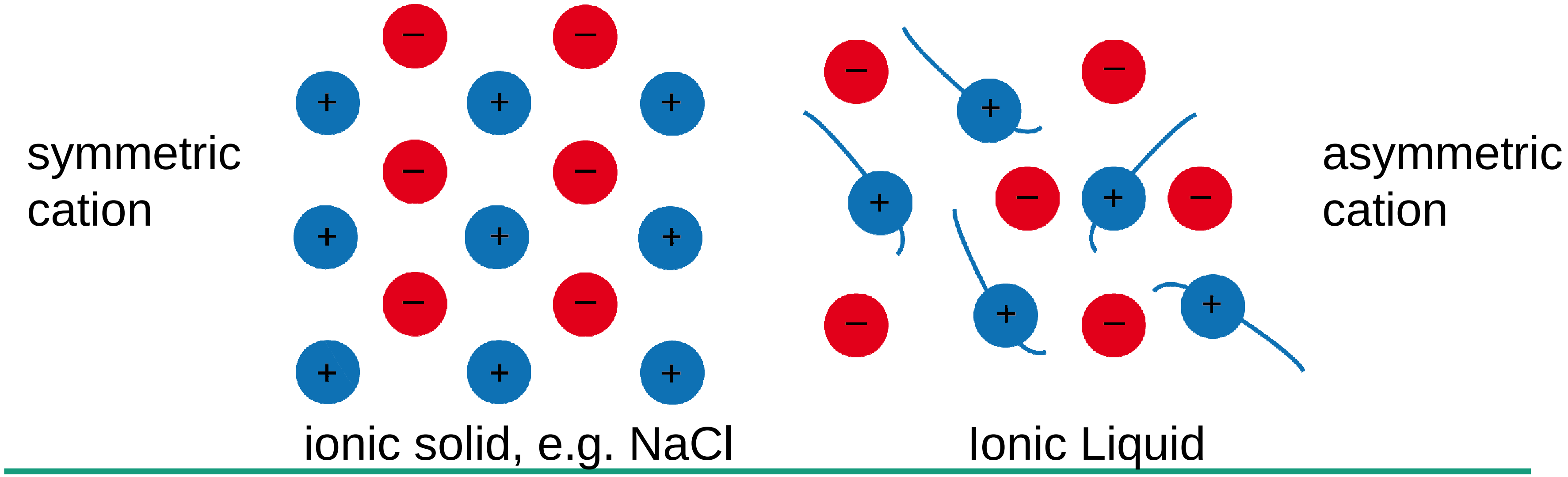


since 1996 exponential growth of scientific publications about ILs

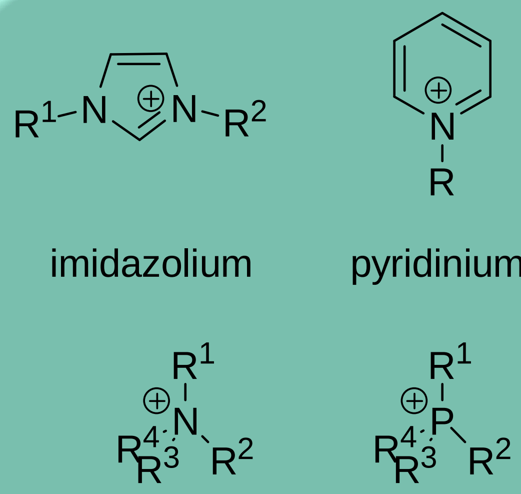
aspects favoring ILs

- organic cation with low structural symmetry

  (e.g. asymmetric imidazolium cation)
- weak intermolecular interactions
- anion with diffuse negative charge



commercial ILs



imidazolium pyridinium

ammonium phosphonium

PF_6^- BF_4^- $R_2PO_2^-$ NO_3^- Cl^- Br^- I^-

$alkylSO_4^-$ triflate tosylate acetate

$NC{-}N^{-}{-}CN$ $B(CN)_4^-$ SCN^- $[AlCl_4]^-$...

all relevant properties are determined by anion AND cation

10^{18} possible ILs

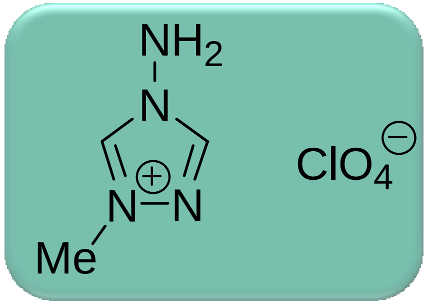
3000 described in literature

300 commercial available

results and potential applications

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

		AMTP
impact sensitivity	[Nm]	7.5
friction sensitivity	[N]	64
melting point	[℃]	+84
decomposition temperature	[℃]	+259

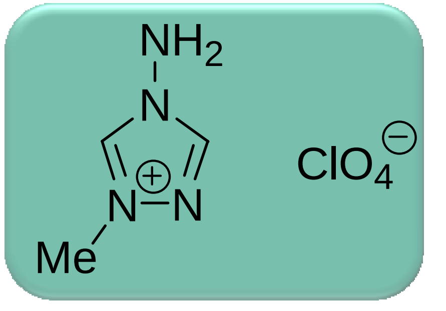


→ component in melt cast formulations

results and potential applications

- 4-amino-1-methyl-1,2,4-triazolium perchlorate (AMTP)
  - comparison to TNT

		TNT	AMTP
melting point	[℃]	80	84
decomposition temperature[a]	[℃]	253	290
oxygen balance	[%]	-74	-44
heat of explosion[b]	[J/g]	3766	4096
shock velocity[c]]	[m/s]	6886	7287



[a] DSC onset; heating rate 5 K/min. [b] calculated with ICT Code water liquid. [c] calculated with CHEETAH 2.0.

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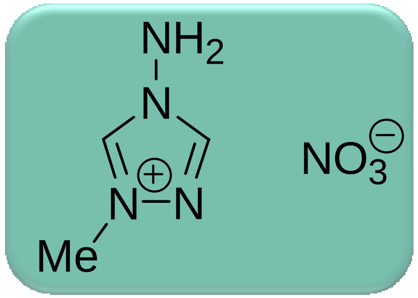
EILs – Energetic Ionic Liquids

- requirements for EILs:
  - liquid between
    -40 °C and +150 °C
  - energetic
  - long-term stable
  - insensitive

results and potential applications

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

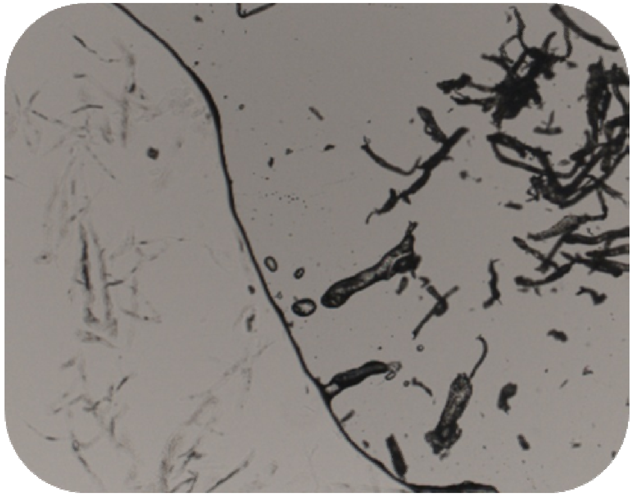
		AMTN
impact sensitivity	[Nm]	15
friction sensitivity	[N]	144
glass transition temperature	[℃]	-55
decomposition temperature	[℃]	+259



→ wide operating temperature range

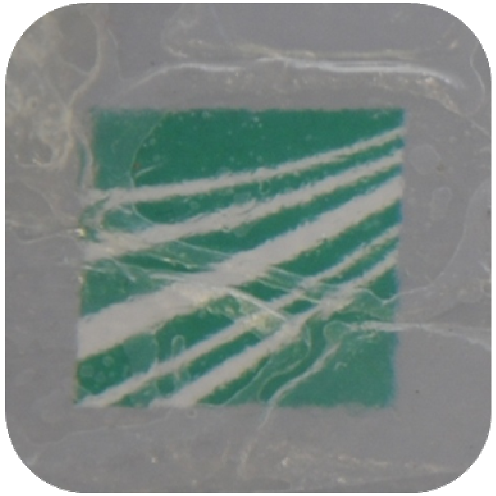
results and potential applications

- 4-amino-1-methyl-1,2,4-triazolium nitrate (AMTN)
  - gelatinization of nitrocellulose (N = 12.6%)



microscopic picture
of gelatinized NC

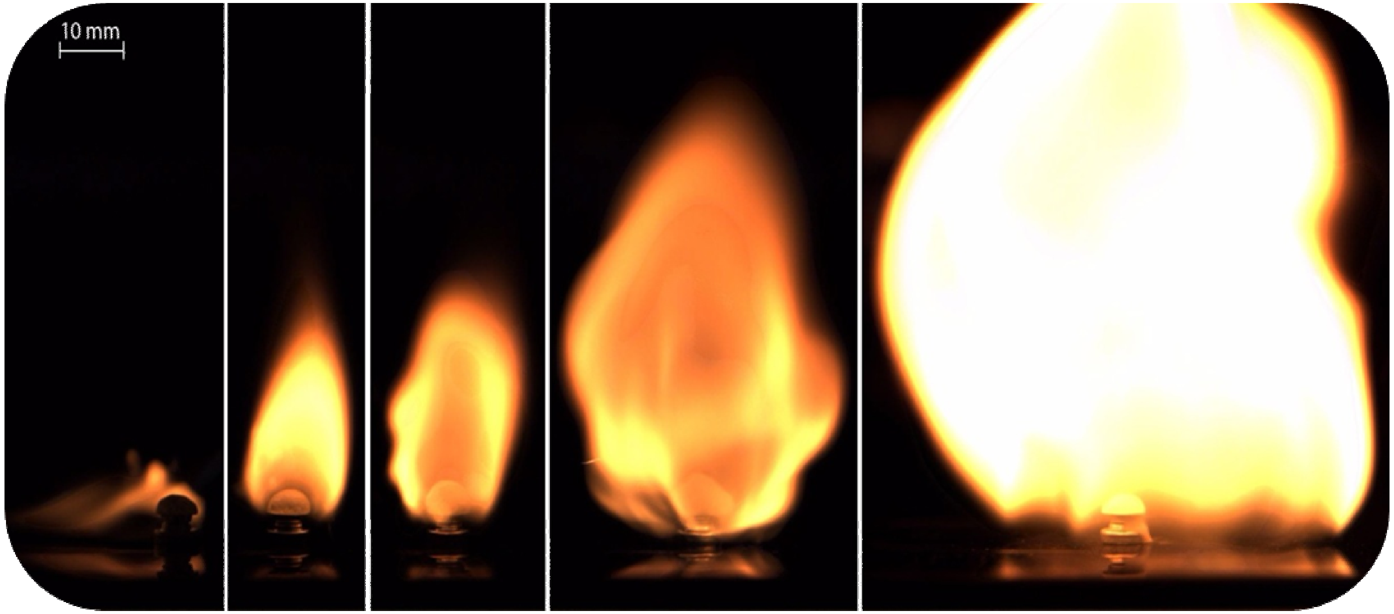
film of NC / AMTN (1:4)



transparency of film

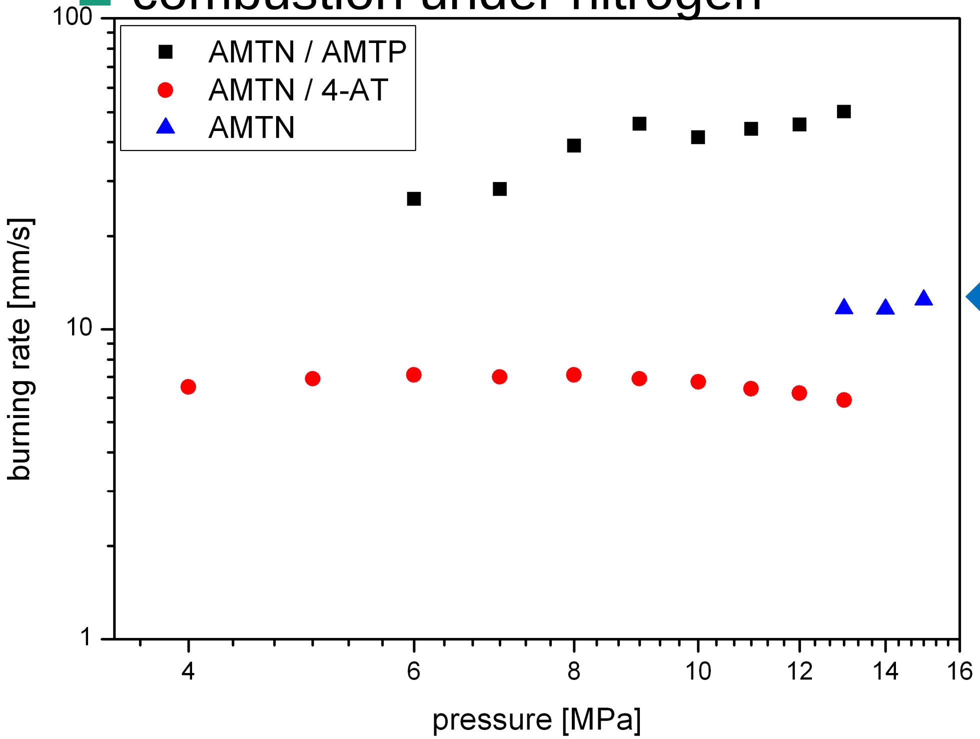
results and potential applications

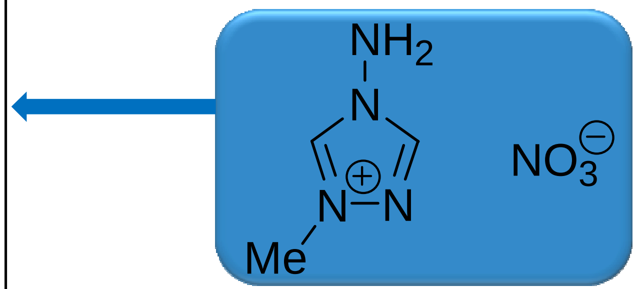
- 4-amino-1-methyl-1,2,4-triazolium nitrate (AMTN)
  - combustion in atmospheric air



results and potential applications

- 4-amino-1-methyl-1,2,4-triazolium nitrate (AMTN)
  - combustion under nitrogen

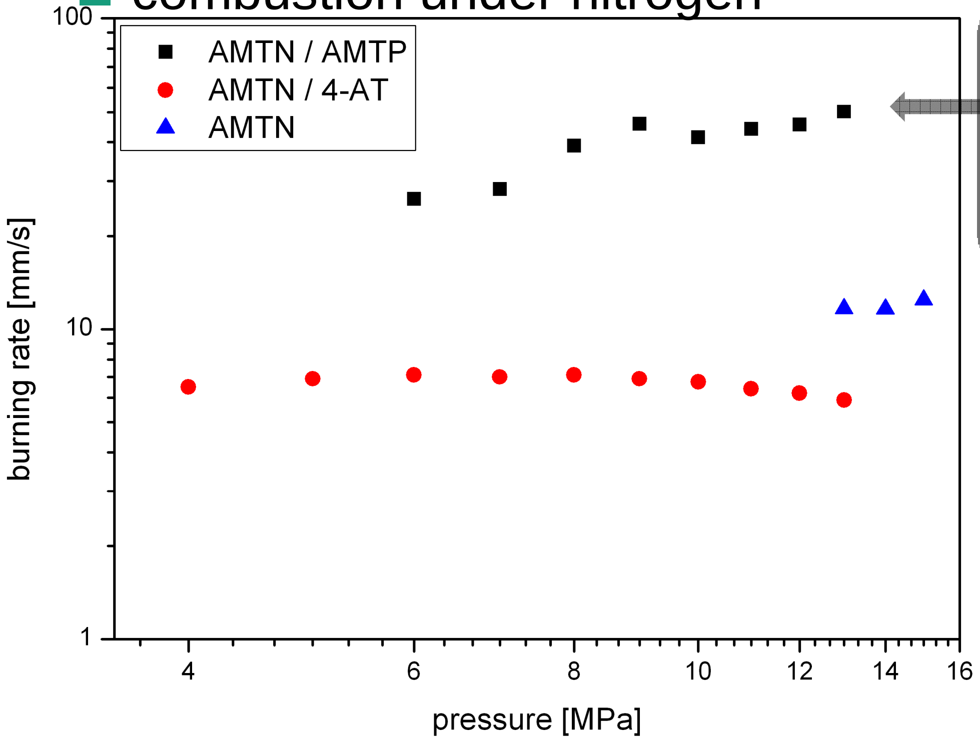


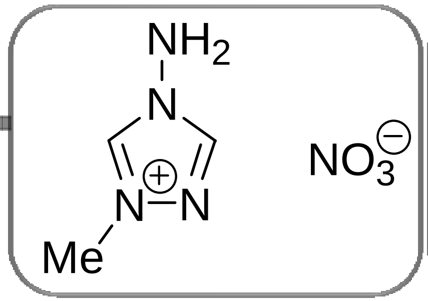


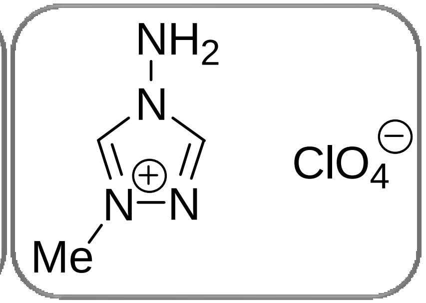
no combustion at lower pressures

results and potential applications

- 4-amino-1-methyl-1,2,4-triazolium nitrate (AMTN)
  - combustion under nitrogen

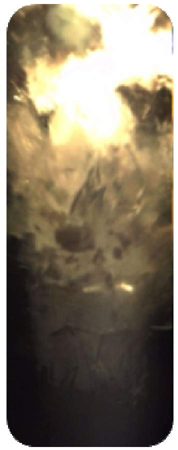






94 / 6 wt%

deflagration of
pure AMTP



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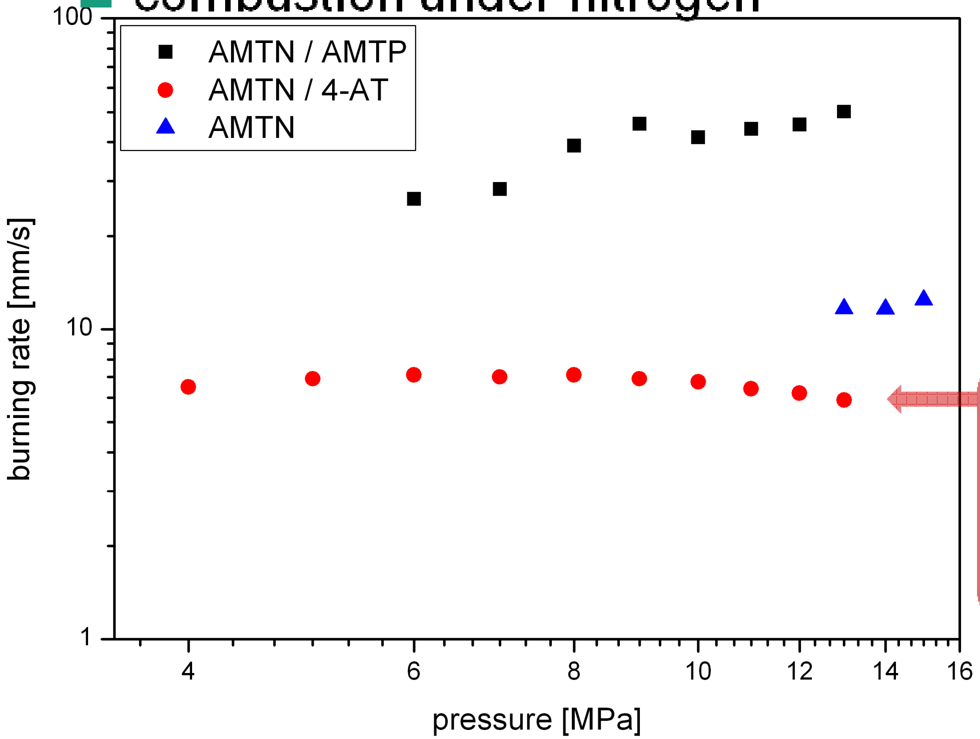
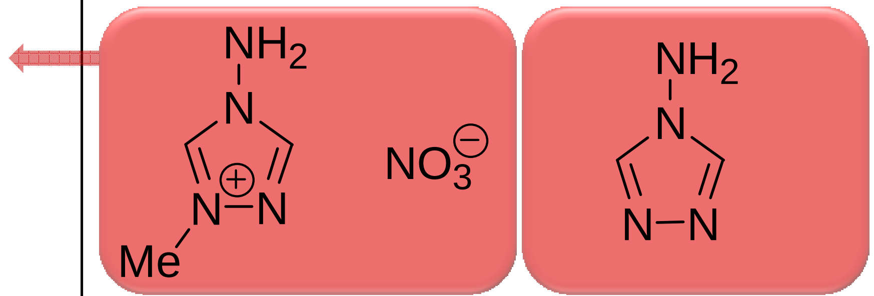
results and potential applications

- 4-amino-1-methyl-1,2,4-triazolium nitrate (AMTN)
  - combustion under nitrogen



fuel mixture



66 / 34 wt%

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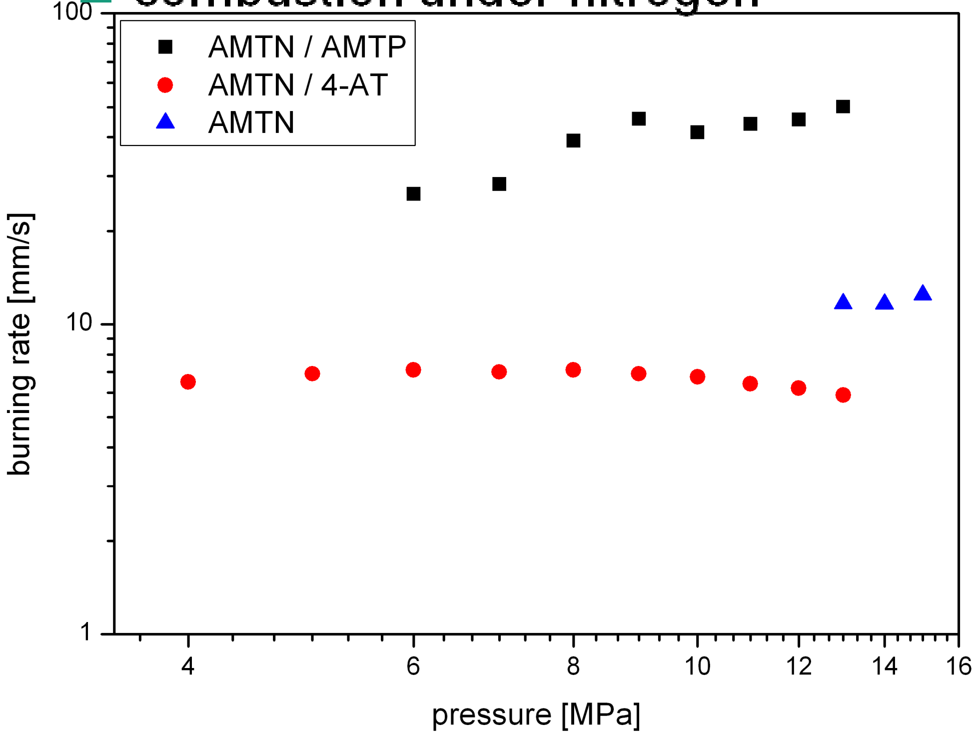
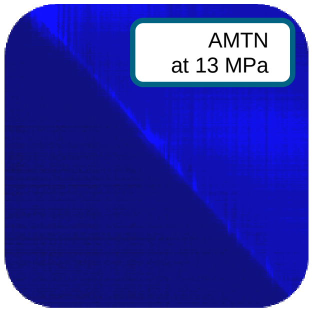
results and potential applications

- 4-amino-1-methyl-1,2,4-triazolium nitrate (AMTN)
  - combustion under nitrogen



linear regression rate



regression image

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results and potential applications

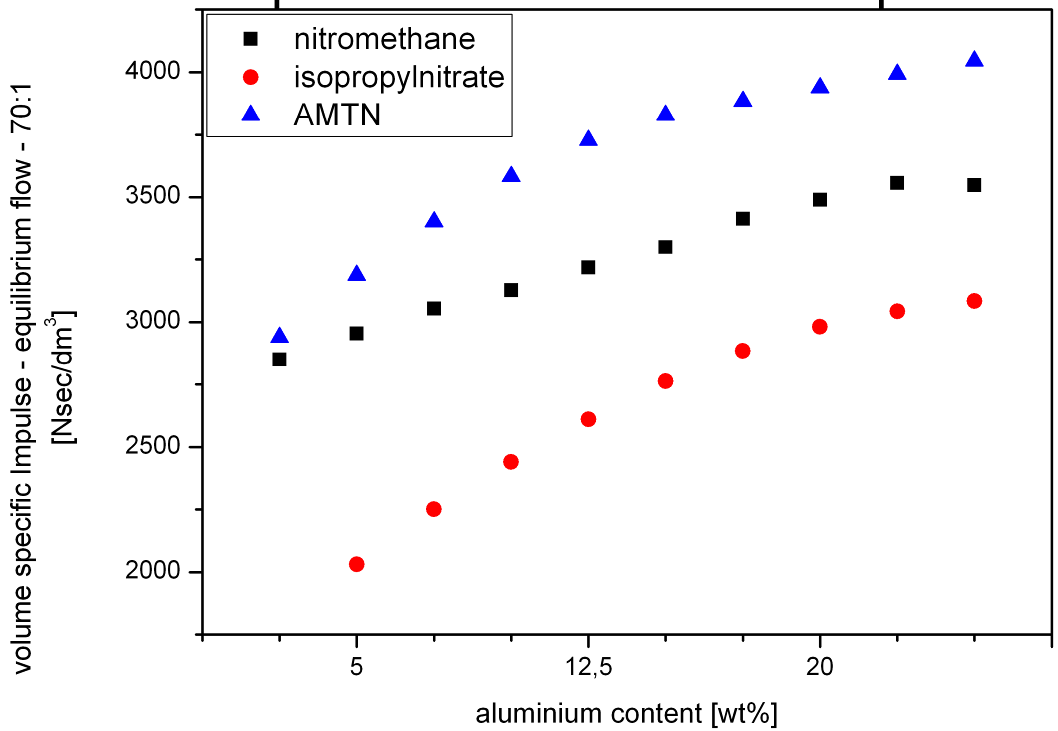
- 4-amino-1-methyl-1,2,4-triazolium nitrate (AMTN)
  - comparison to conventional liquid energetic materials

	melting point	boiling point	density	vapor pressure
	[℃]	[℃]	[g/cm ^{3}]	[kPa]
nitromethane	-28	101	1.14	4.8
isopropylnitrate	-82	100	1.03	3.5
AMTN	-55[a]	T_{dec} > 200	1.44	< 0.001

[a] glass transition temperature

results and potential applications

- 4-amino-1-methyl-1,2,4-triazolium nitrate (AMTN)
  - comparison to conventional liquid energetic materials



potential high density powerful propellant

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outlook

performance

thermal stability mechanical sensitivity

freezing point oxygen balance

enthalpy of formation

wide variety of anion and cation combination possibilities

tailoring possible

task specific EILs

summary and conclusion

EILs – Energetic Ionic Liquids

- relative new research area

- improved physical properties in comparison to conventional energetic materials

- increased performance possible

- very low toxicity of the vapor phase

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Thank you