

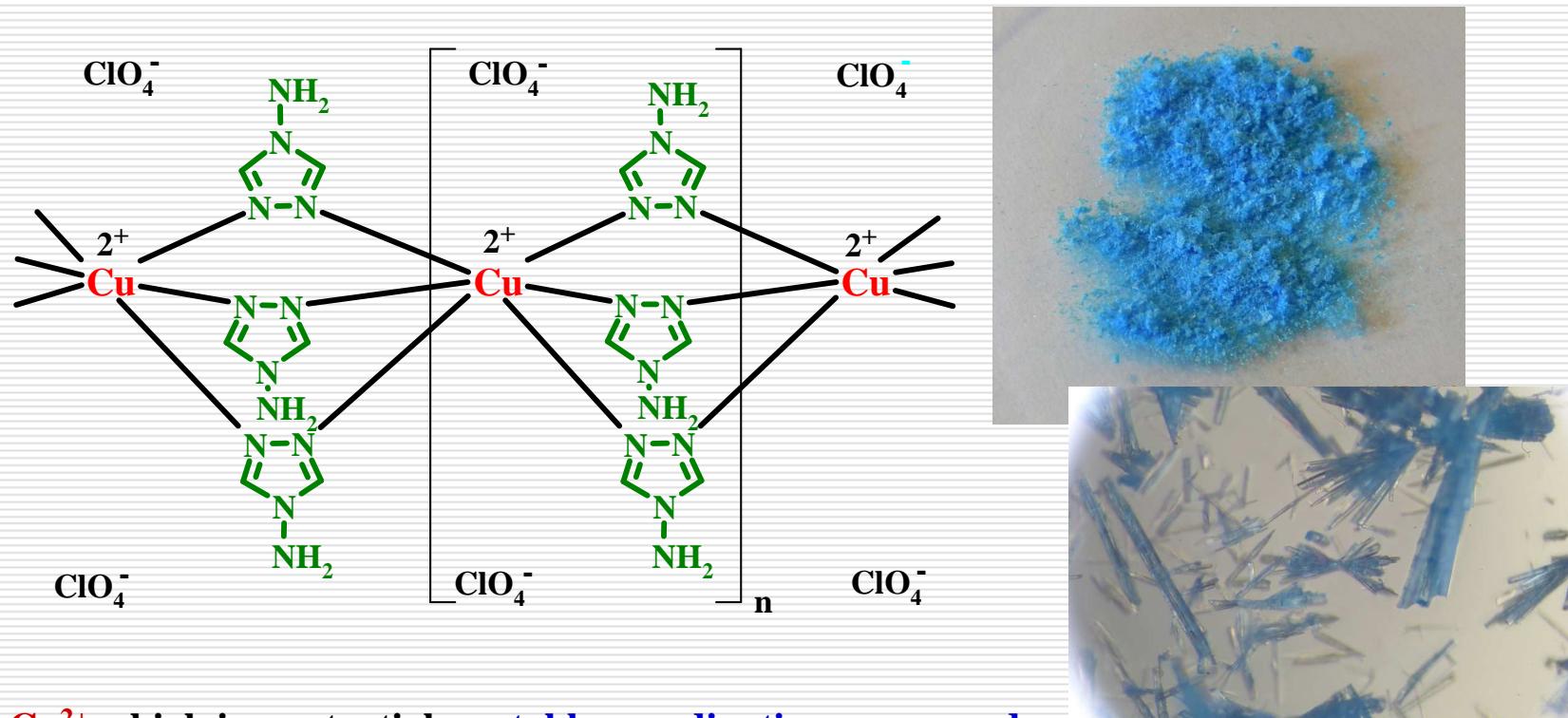
Detonation and decomposition characteristics of dichlorate(VII) μ -tris(4-amino-1,2,4-triazole)copper(II)



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Presentation of $\{[\text{Cu}(\text{C}_2\text{H}_4\text{N}_4)_3](\text{ClO}_4)_2\}_n$



Cu^{2+} – high ion potential \Rightarrow stable coordination compounds

ClO_4^- – oxygen rich and high redox potential \Rightarrow high initiating performance

4-Amino-1,2,4-triazole – stable compound and didentate, bridging ligand \Rightarrow complex stability

Presentation of $\{[\text{Cu}(\text{C}_2\text{H}_4\text{N}_4)_3](\text{ClO}_4)_2\}_n$

- + it is a moderate sensitive to mechanical stimuli (10 N, 1 J) and thermally resistant detonator (it decomposes above 250 °C),
- + spark ignition threshold of the bulk powder is ca. 33 mJ (LA 0.1 μJ and RDX 200 mJ),
- + it detonates upon exposure to flame and initiates detonation of PETN/RDX/HMX charges (minimal priming charge 150 mg),
- + it can be used as an environmentally friendly and safe replacement of lead azide and lead styphnate.

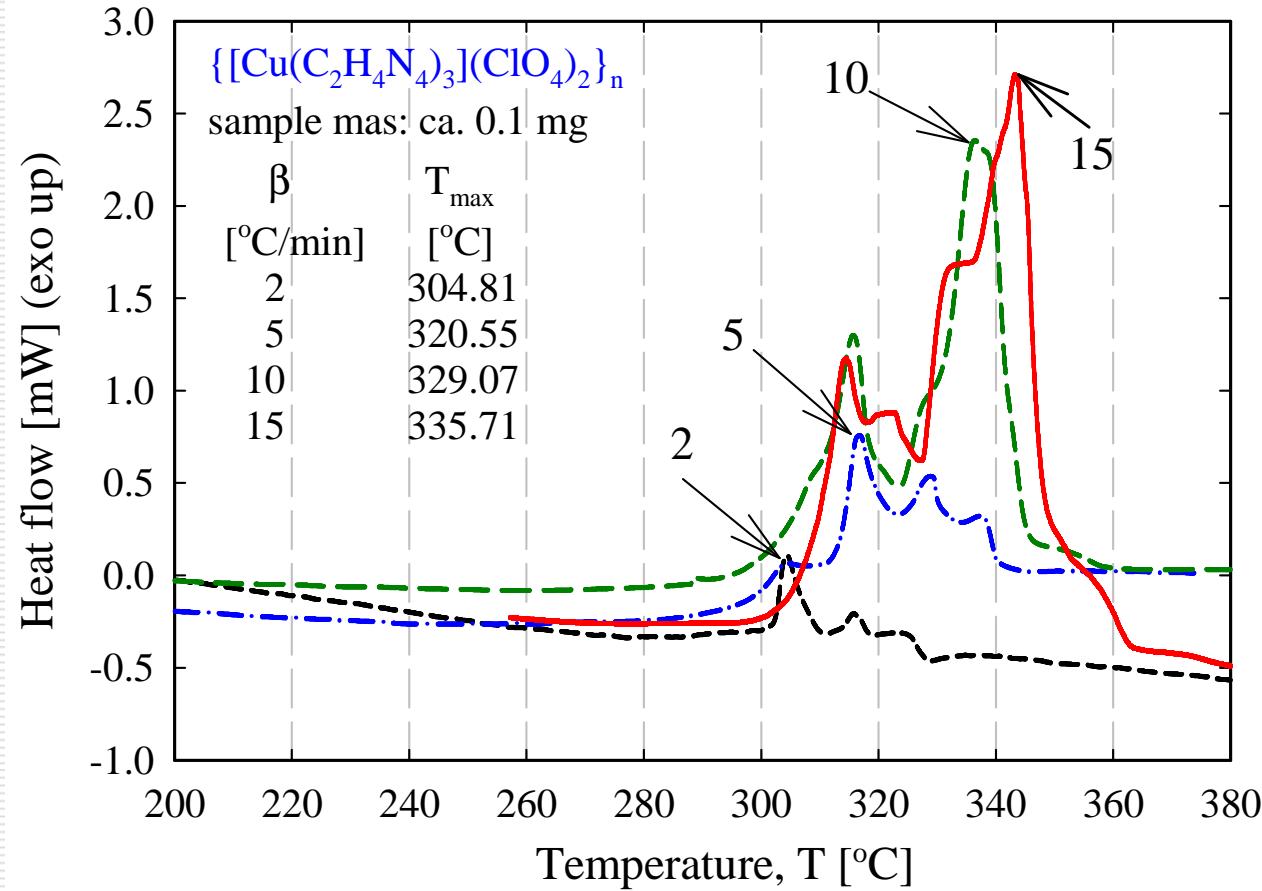


Fuse and electric blasting caps



Percussion primers

Non-isothermal kinetics analysis



Arrhenius equation:

$$\ln k = 25.93 - \frac{182600}{RT}$$

Thermodynamic aspects

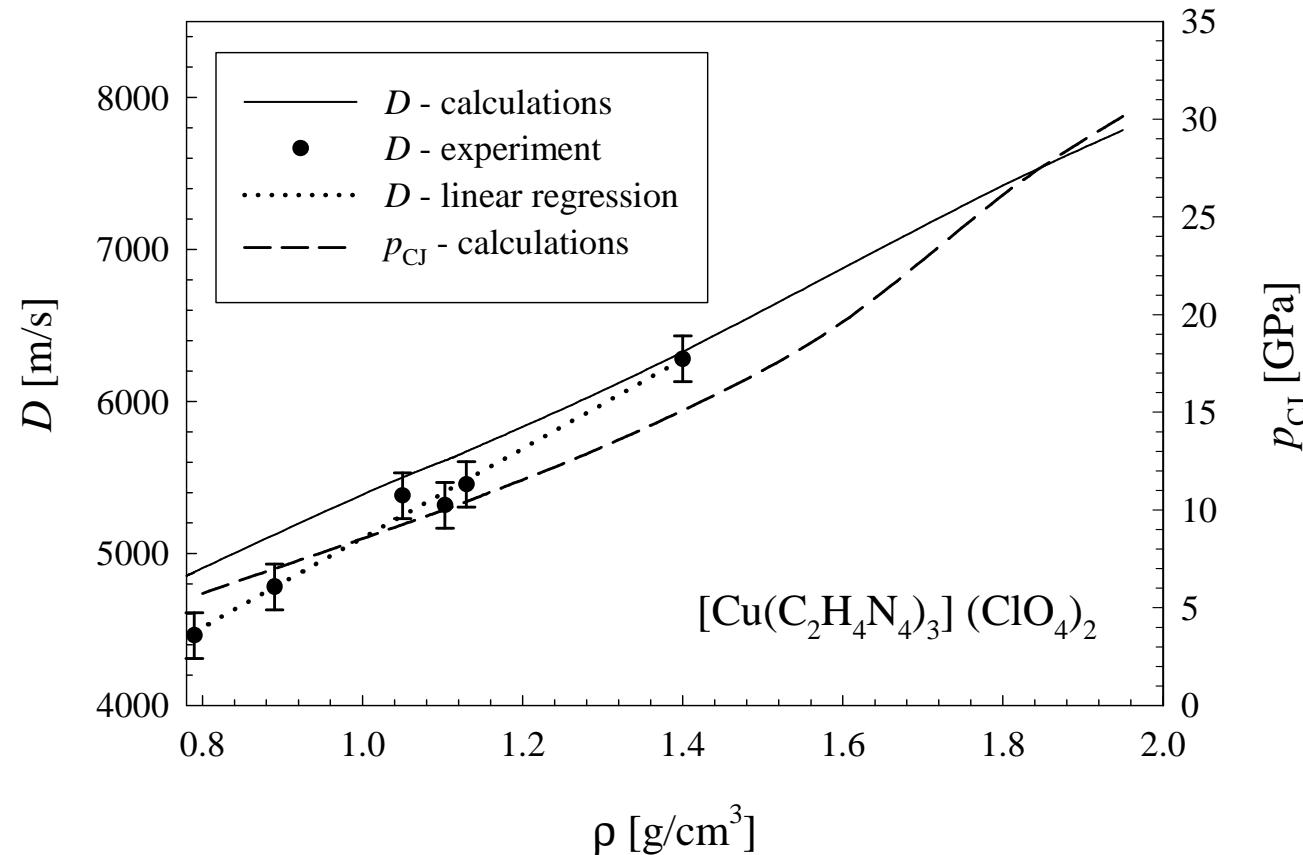


Physicochemical properties of $\{[\text{Cu}(\text{C}_2\text{H}_4\text{N}_4)_3](\text{ClO}_4)_2\}_n$

Formula	$\text{C}_6\text{H}_{12}\text{O}_8\text{N}_{12}\text{Cl}_2\text{Cu}$
Molar mass [g/mol]	514.69
Nitrogen content [%]	32.66
Oxygen balance [%]	-27.98
Activation energy [kJ/mol]	182.6
Heat of explosion in Ar [kJ/kg]	3850 ± 70 (calc. 4204)
Heat of explosion in O₂ [kJ/kg]	9600 ± 300
Enthalpy of formation [kJ/mol]	801.5

Detonation parameters

CHEETAH code, BKW EOS, Formation enthalpy: 801.5 kJ/mol



Dependence of detonation velocity and detonation pressure on density

Calculated $D@p_0$

7720@1.96

Calculated $p_{CJ}@p_0$

30.5@1.96

Measured $D@p_0$

2900@0.25

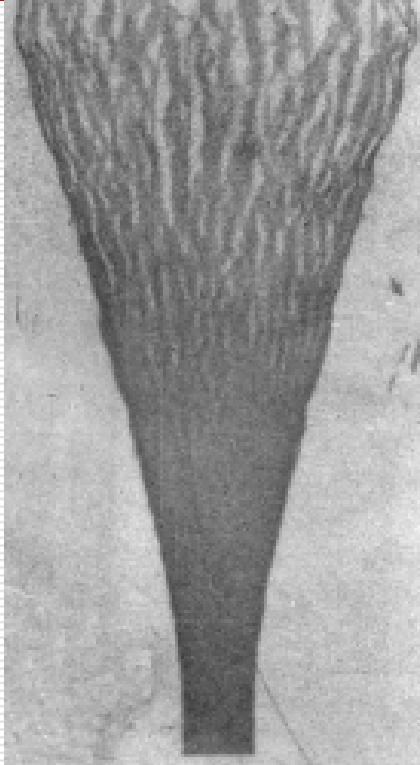
4470@0.79

4780@0.89

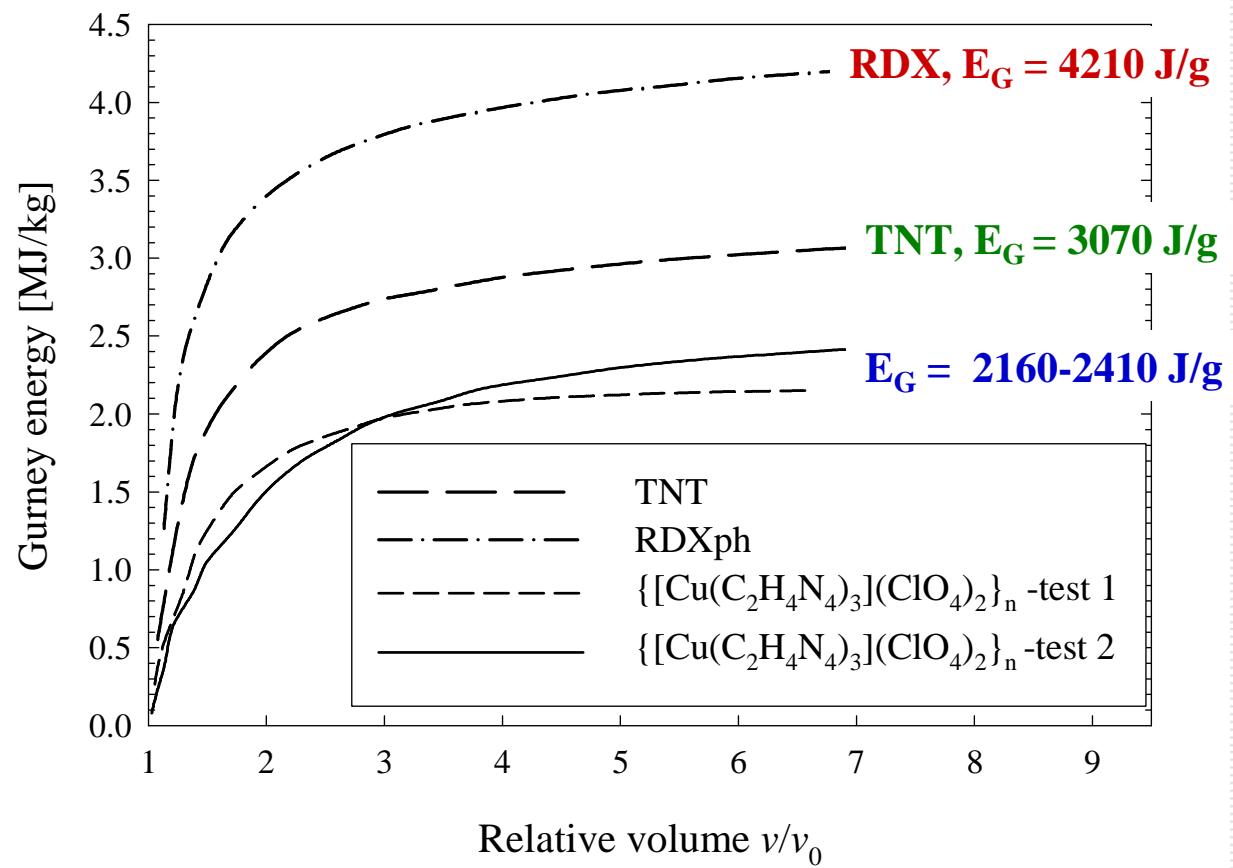
5380@1.05

6280@1.40

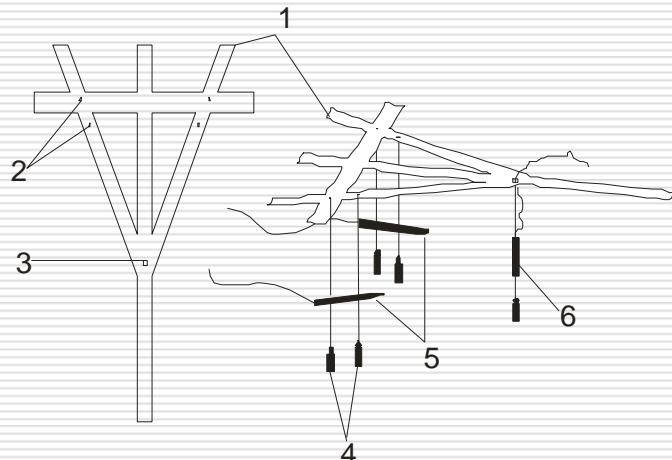
Cylinder test results



Copper tube
Length: 200 mm
Diameter: 15/13 mm



Underwater test results

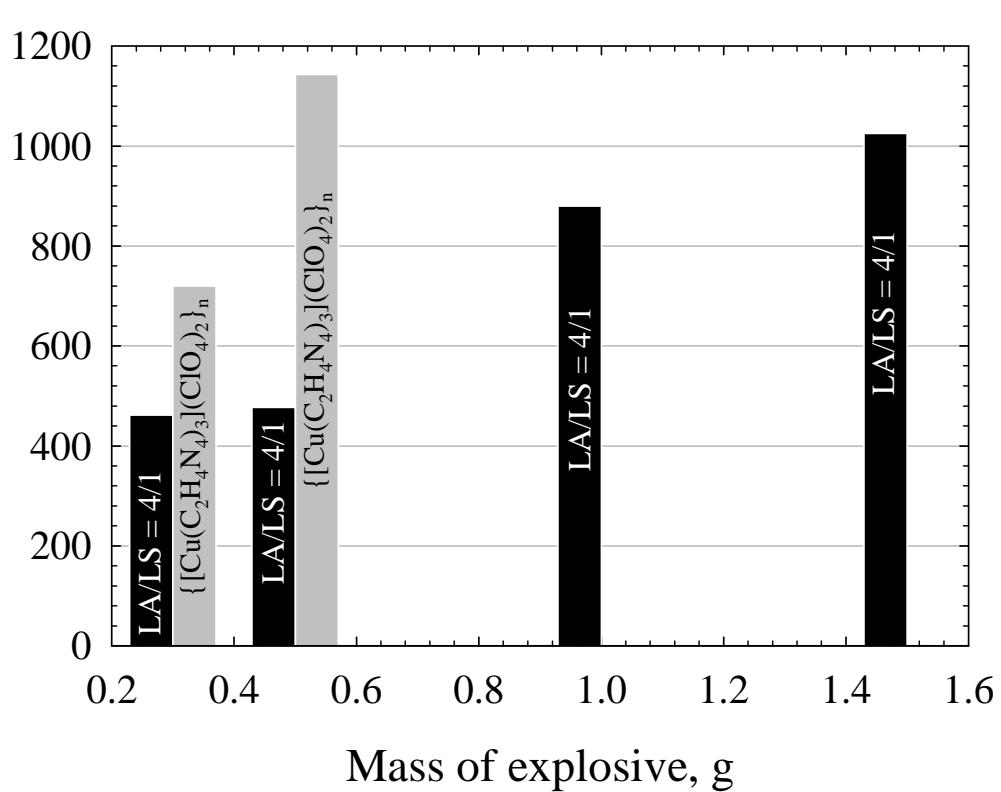


5 – pressure sensors,
6 – tested detonator



Lead block test
323 cm³/10g
0.7 g/cm³

Total energy, $E = E_S + E_b$, J



Heat of detonation: 1600 (LA/LS) and 3850 kJ/kg
Volume of gas products: 240 (LA/LS) and 800 dm³/kg

Summary

Dichlorate(VII) μ -tris(4-amino-1,2,4-triazole)copper(II) is a thermally stable compound – while heating it explosively decomposes above 300 °C and the activation energy of decomposition is ca. 183 kJ/mole

The heat of explosion equals to ca. 3850 kJ/kg, and it detonates at 6.3 km/s in unconfined charges pressed to a density of 1.4 g/cm³. Its acceleration ability (the Gurney energy ca. 2300 J/g) is lower by a factor of 1.5÷2 than that of high explosives.

The performance of $\{[Cu(C_2H_4N_4)_3](ClO_4)_2\}_n$ is very high as for primary explosive. In underwater detonation tests, it produces comparable effects as charges of LA/LS mixture with masses higher by a factor of 2.5÷3.
