Investigation of the micellization process of newly synthesized surface-active caffeine-based compounds in aqueous solutions

Network for Equilibria and Chemical Thermodynamics Advanced Research
COST ACTION 18202

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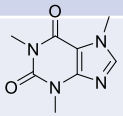
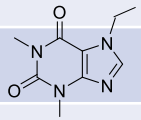
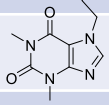
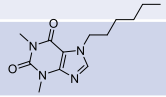
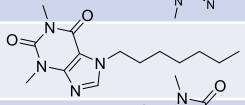
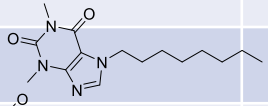
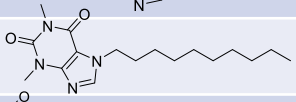
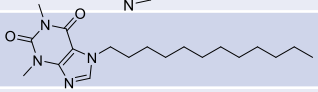
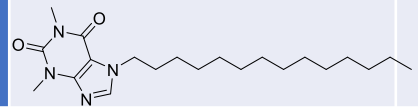
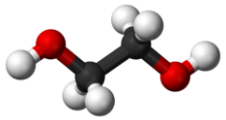
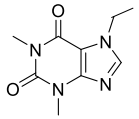
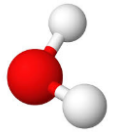
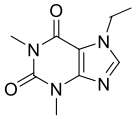
Structures of the synthetised of caffeine-based compounds

Atmosfere N2	Heating rate 10 C/min	
Range	Room temperature to 450 C – thermogravimetry (TG)	
Name	Structure	*T* decomposition
Theophylline		299
Caffeine (N-methyl theophylline)		280
N-ethyl-theophylline		230
N-butyl-theophylline		213
N-hexyl-theophylline	 LIQUID	290
N-heptyl-theophylline	 LIQUID	284
N-octyl-theophylline		277
N-decyl-theophylline		304
N-dodecyl-theophylline		346
N-tetradecyl-theophylline		355

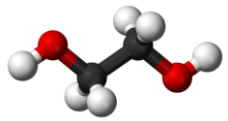
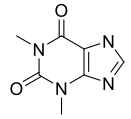
Selected systems (caffeine-based compound in solvent)

 and  → *m* = 0.0125-0.125 mol/kg

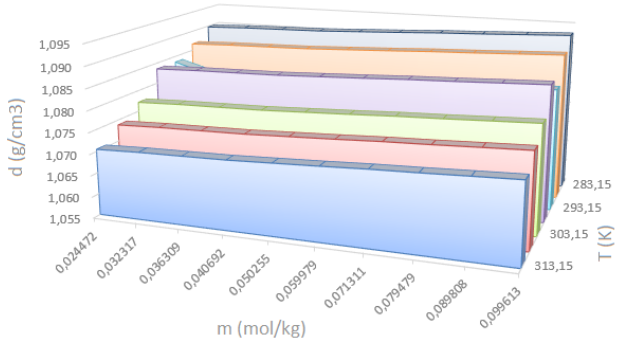
Ethylene glycol — N-ethyl- theophylline

 and  → *m* = 0.025-0.200 mol/kg

water — N-ethyl- theophylline

  → *m* = 0.020-0.100 mol/kg

Ethylene glycol — theohylline



Methods:

Synthesis
Thermal properties
DSC (differential scanning calorimetry)
Density
Viscosity