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## Thermochemistry of ammonium based ionic liquids: Thiocyanates - Experiments and computations

Yermalayeu A., Zaitsau D., Emel'yanenko V., Verevkin S.  
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

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### Abstract

© Springer Science+Business Media New York 2015. Abstract Molar enthalpies of solution of tetra-n-butylammonium thiocyanate  $[N(\text{Bu})_4][\text{SCN}]$  and tetra-n-pentylammonium thiocyanate  $[N(\text{Pe})_4][\text{SCN}]$  in water were measured by using solution calorimetry. The enthalpy of combustion of  $[N(\text{Bu})_4][\text{SCN}]$  was measured by using rotation bomb combustion calorimetry and the enthalpy of formation of this ionic liquids was derived. The thermal behavior of  $[N(\text{Bu})_4][\text{SCN}]$  was studied using differential scanning calorimetry. Quantum-chemical calculations of the molar enthalpy of formation in the gaseous phase have been performed for the series  $[N(\text{R})_4][\text{SCN}]$  with  $\text{R} = (\text{Me}, \text{Et}, \text{n-Bu}, \text{and n-Pe})$  using the G3MP2 level of theory. Experimental and calculated values of the enthalpies of formation are in agreement within the boundaries of the experimental uncertainties.

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### Keywords

Combustion calorimetry, Enthalpy of formation, Enthalpy of solution, Ionic liquids, Quantum-chemical calculations, Solution calorimetry